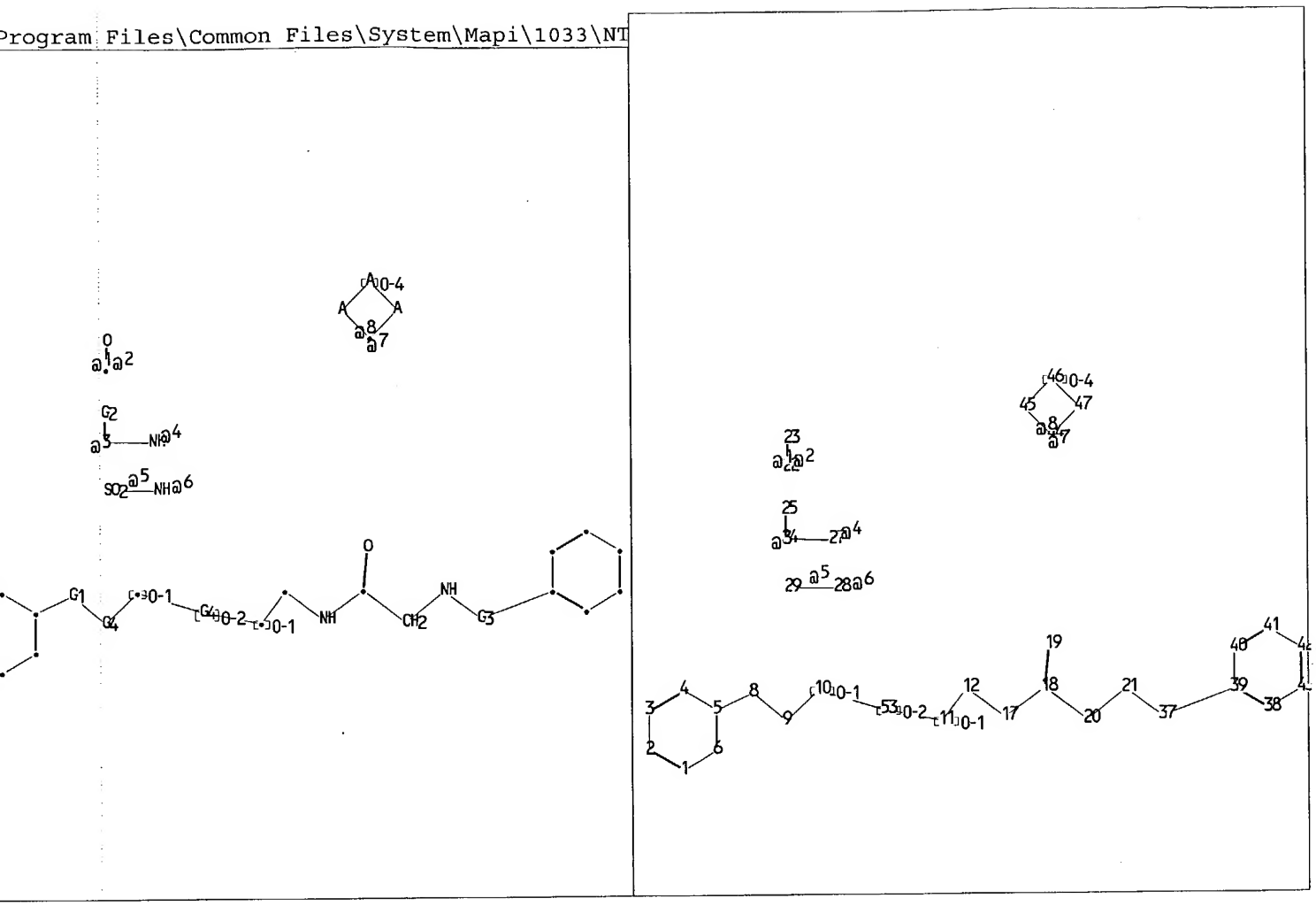
Program Files\Common Files\System\Mapi\1033\NT



in nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53
g nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47
in bonds :
5-8 8-9 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37 22-23 24-25
24-27 28-29 37-39
g bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 44-45 44-47 45-46
46-47
ct/norm bonds :
5-8 8-9 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27 28-29 37-39
44-45 44-47 45-46 46-47
ct bonds :
11-12 18-20 20-21
malized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

O,N

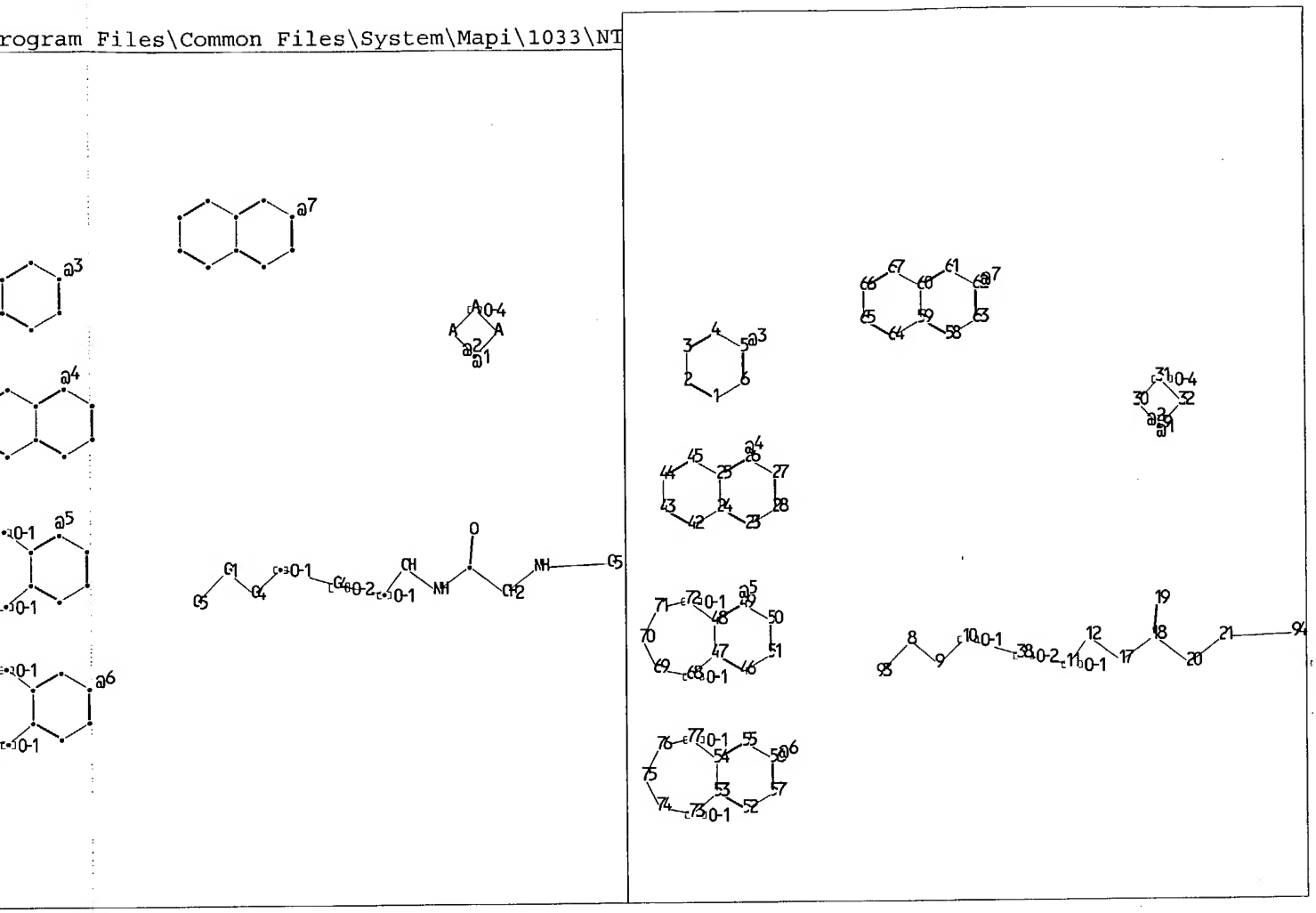
O,S

SO2,[*1-*2],[*3-*4],[*5-*6]

C,[*7-*8]

ch level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 27:CLASS 28:CLASS 29:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 53:CLASS

rogram Files\Common Files\System\Mapi\1033\NT



n nodes :
8 9 10 11 12 17 18 19 20 21 38 93 94
g nodes :
1 2 3 4 5 6 23 24 25 26 27 28 29 30 31 32 42 43 44 45 46 47 48 49
50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72
73 74 75 76 77
in bonds :
8-9 8-93 9-10 10-38 11-12 11-38 12-17 17-18 18-19 18-20 20-21 21-94
g bonds :
1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 24-42 25-26 25-45 26-27 27-28 29-30
29-32 30-31 31-32 42-43 43-44 44-45 46-47 46-51 47-48 47-68 48-49 48-72 49-50
50-51 52-53 52-57 53-54 53-73 54-55 54-77 55-56 56-57 58-59 58-63 59-60 59-64
60-61 60-67 61-62 62-63 64-65 65-66 66-67 68-69 69-70 70-71 71-72 73-74 74-75
75-76 76-77
ct/norm bonds :
8-9 8-93 9-10 10-38 11-38 12-17 17-18 18-19 21-94 29-30 29-32 30-31 31-32
ct bonds :
11-12 18-20 20-21 47-68 48-72 53-73 54-77 68-69 69-70 70-71 71-72 73-74 74-75
75-76 76-77
malized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 24-42 25-26 25-45 26-27 27-28 42-43
43-44 44-45 46-47 46-51 47-48 48-49 49-50 50-51 52-53 52-57 53-54 54-55 55-56
56-57 58-59 58-63 59-60 59-64 60-61 60-67 61-62 62-63 64-65 65-66 66-67
lated ring systems :
containing 1 : 23 : 46 : 52 : 58 :

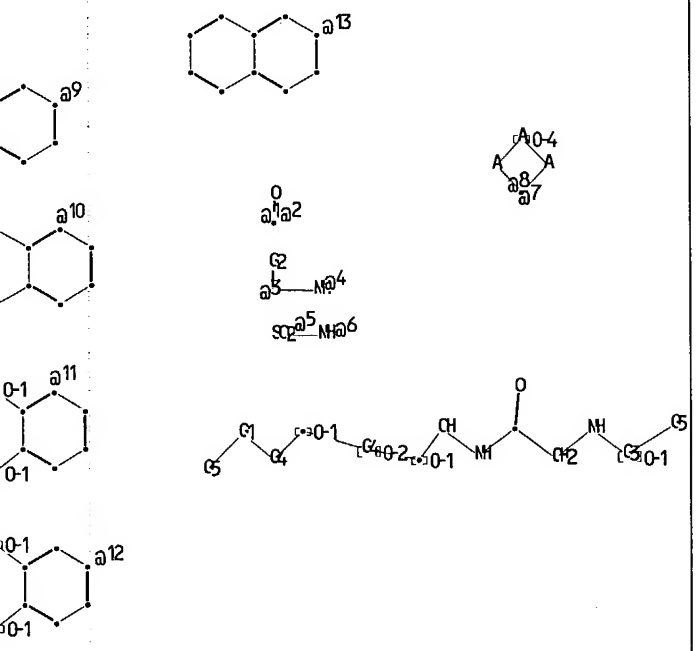
O,N

O,S

CH,[*1-*2]

```
3], [*4], [*5], [*6], [*7]

 level :
:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS  11:CLASS
2:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  23:Atom  24:Atom  25:Atom
6:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  38:CLASS  42:Atom  43:Atom
4:Atom  45:Atom  46:Atom  47:Atom  48:Atom  49:Atom  50:Atom  51:Atom  52:Atom  53:Atom
4:Atom  55:Atom  56:Atom  57:Atom  58:Atom  59:Atom  60:Atom  61:Atom  62:Atom  63:Atom
4:Atom  65:Atom  66:Atom  67:Atom  68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom
4:Atom  75:Atom  76:Atom  77:Atom  93:CLASS  94:CLASS
```

ogram Files\Common Files\System\Mapi\1033\NT



n nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55 110 111
nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49 59 60 61 62 63 64 65 66
67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89
90 91 92 93 94
n bonds :
8-9 8-110 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37 22-23
24-25 24-27 28-29 37-111
bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-59 40-41 40-62 41-42 42-43 46-47
46-49 47-48 48-49 59-60 60-61 61-62 63-64 63-68 64-65 64-85 65-66 65-89 66-67
67-68 69-70 69-74 70-71 70-90 71-72 71-94 72-73 73-74 75-76 75-80 76-77 76-81
77-78 77-84 78-79 79-80 81-82 82-83 83-84 85-86 86-87 87-88 88-89 90-91 91-92
92-93 93-94
c/norm bonds :
8-9 8-110 9-10 10-55 11-55 12-17 17-18 18-19 21-37 22-23 24-25 24-27 28-29
37-111 46-47 46-49 47-48 48-49
c bonds :
11-12 18-20 20-21 64-85 65-89 70-90 71-94 85-86 86-87 87-88 88-89 90-91 91-92
92-93 93-94
alized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-59 40-41 40-62 41-42 42-43 59-60
60-61 61-62 63-64 63-68 64-65 65-66 66-67 67-68 69-70 69-74 70-71 71-72 72-73
73-74 75-76 75-80 76-77 76-81 77-78 77-84 78-79 79-80 81-82 82-83 83-84
ated ring systems :
containing 1 : 38 : 63 : 69 : 75 :

N

S

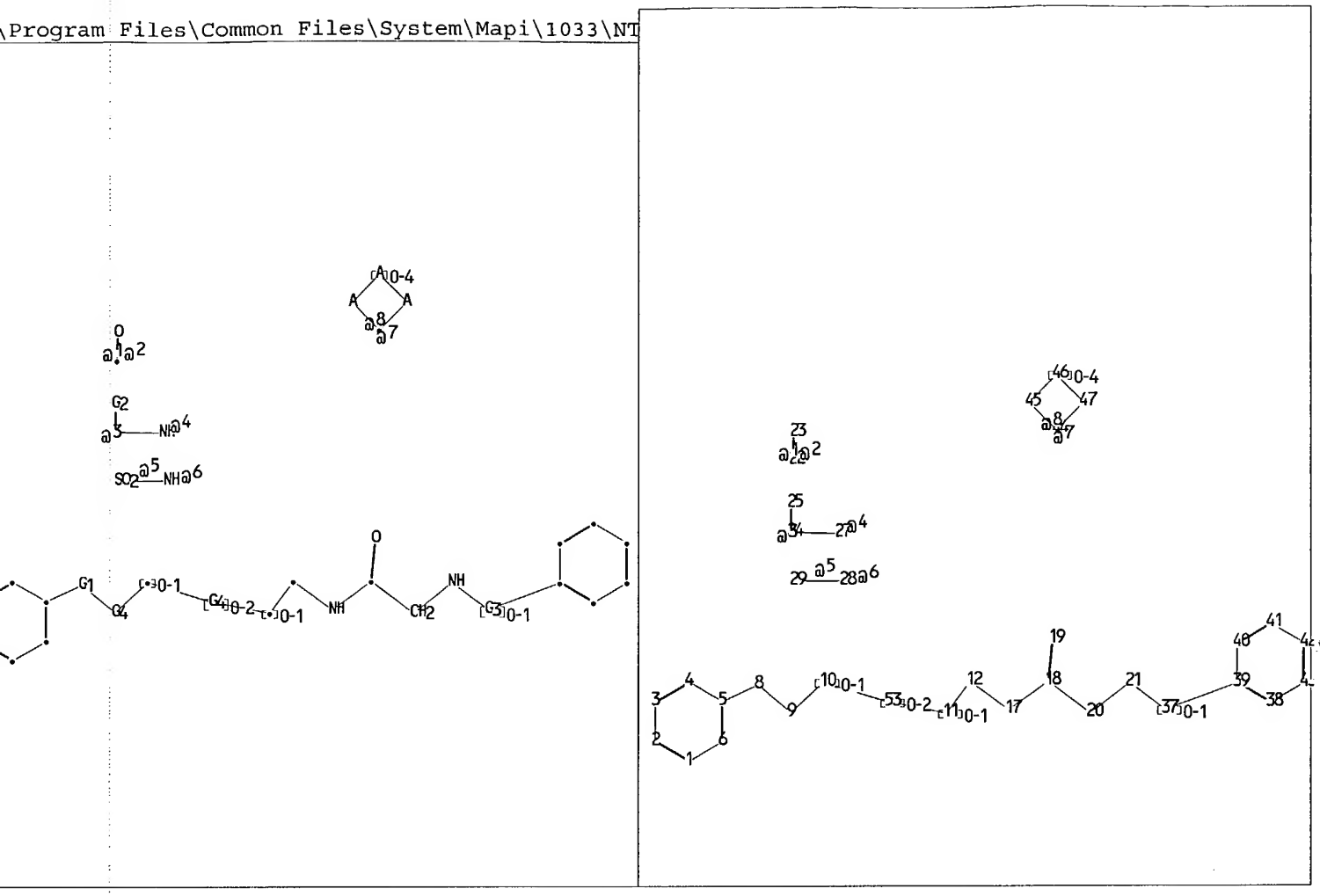
3:SO2,[*1-*2],[*3-*4],[*5-*6]

4:CH,[*7-*8]

5:[*9],[*10],[*11],[*12],[*13]

atch level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 27:CLASS 28:CLASS 29:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 46:Atom 47:Atom 48:Atom 49:Atom 55:CLASS 59:Atom 60:Atom 61:Atom
62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom
72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom
82:Atom 83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom
92:Atom 93:Atom 94:Atom 110:CLASS 111:CLASS

\Program Files\Common Files\System\Mapi\1033\NT



ain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53
ng nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47
ain bonds :
5-8 8-9 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37 22-23 24-25
24-27 28-29 37-39
ng bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 44-45 44-47 45-46
46-47
act/norm bonds :
5-8 8-9 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27 28-29 37-39
44-45 44-47 45-46 46-47
act bonds :
11-12 18-20 20-21
rmalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

O,N

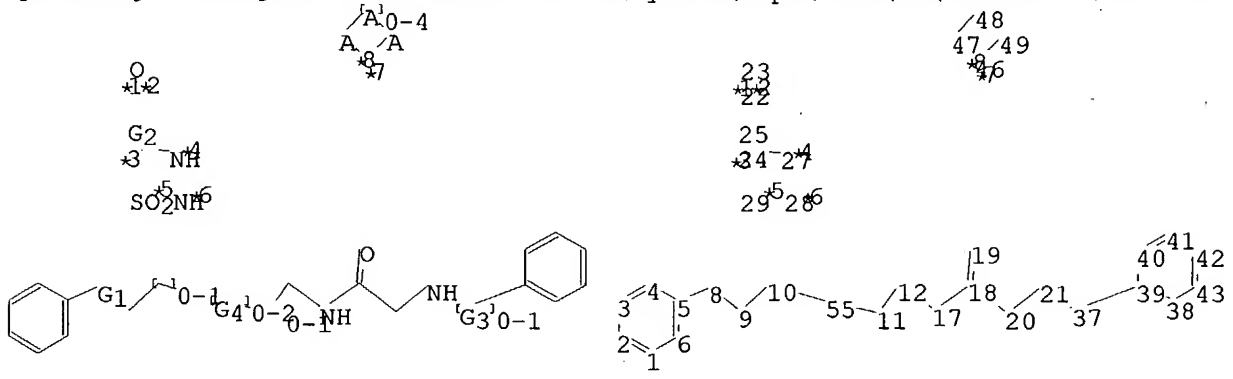
O,S

SO2,[*1-*2],[*3-*4],[*5-*6]

C,[*7-*8]

tch level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS
12:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS
25:CLASS 27:CLASS 28:CLASS 29:CLASS 37:CLASS 38:Atom 39:Atom 40:Atom 41:Atom
42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 53:CLASS

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce).str



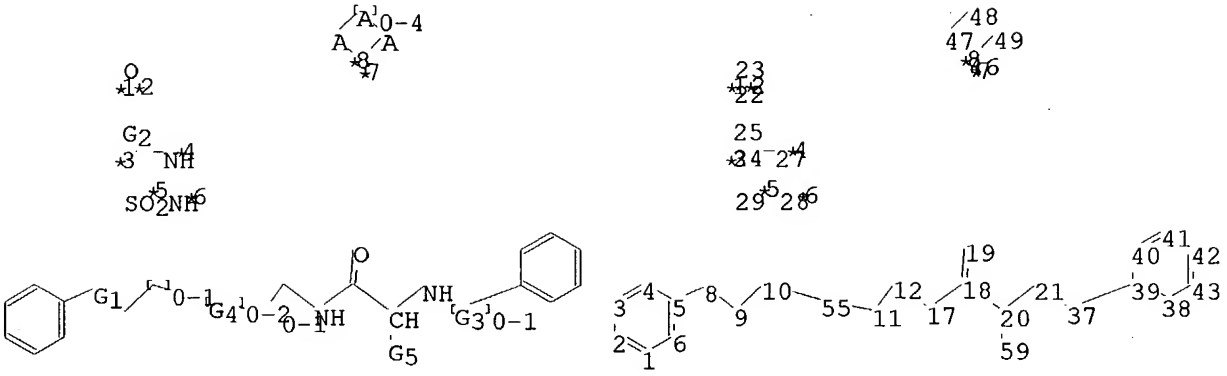
chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49
chain bonds :
5-8 8-9 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 46-47
46-49 47-48 48-49
exact/norm bonds :
5-8 8-9 10-55 11-55 12-17 17-18 18-19 20-21 21-37 22-23 24-25 24-27
28-29 37-39 46-47 46-49 47-48 48-49
exact bonds :
9-10 11-12 18-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

```
G4:C,[*7-*8]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS



L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l1 sss sam
SAMPLE SEARCH INITIATED 16:47:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  23958 TO ITERATE

  4.2% PROCESSED    1000 ITERATIONS                                  1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       469907 TO   488413
PROJECTED ANSWERS:             186 TO      772

L2            1 SEA SSS SAM L1

=> => ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L3    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L4    SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 1).str
```



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55 59
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49
chain bonds :
5-8 8-9 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 20-59
21-37 22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 46-47
46-49 47-48 48-49
exact/norm bonds :
5-8 8-9 10-55 11-55 12-17 17-18 18-19 20-21 20-59 21-37 22-23 24-25
24-27 28-29 37-39 46-47 46-49 47-48 48-49
exact bonds :
9-10 11-12 18-20
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

G1:O,N

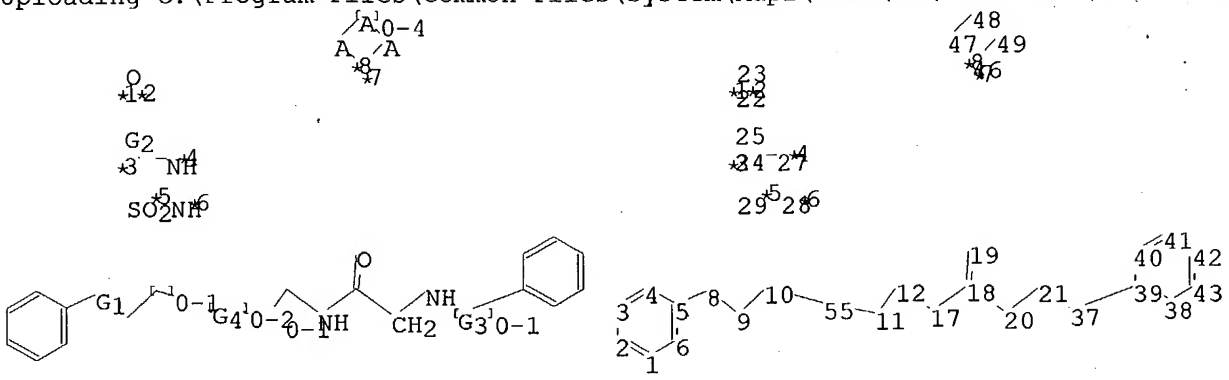
G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:C,[*7-*8]

```
G5:C,H

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS  59:CLASS



L5      STRUCTURE UPLOADED

=> que L5 AND L3 NOT L4

L6   QUE L5 AND L3 NOT L4

=> d l6
L6 HAS NO ANSWERS
L3              SCR 1839
L4              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L5              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L6              QUE  L5 AND L3 NOT L4


=> s l6 sss sam
SAMPLE SEARCH INITIATED 16:50:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  22921 TO ITERATE

  4.4% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       449368 TO   467472
PROJECTED ANSWERS:               0 TO        0

L7            0 SEA SSS SAM L5 AND L3 NOT L4

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L8    SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L9    SCREEN CREATED
```

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 2).str



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49
chain bonds :
5-8 8-9 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 46-47
46-49 47-48 48-49
exact/norm bonds :
5-8 8-9 10-55 11-55 12-17 17-18 18-19 21-37 22-23 24-25 24-27 28-29
37-39 46-47 46-49 47-48 48-49
exact bonds :
9-10 11-12 18-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

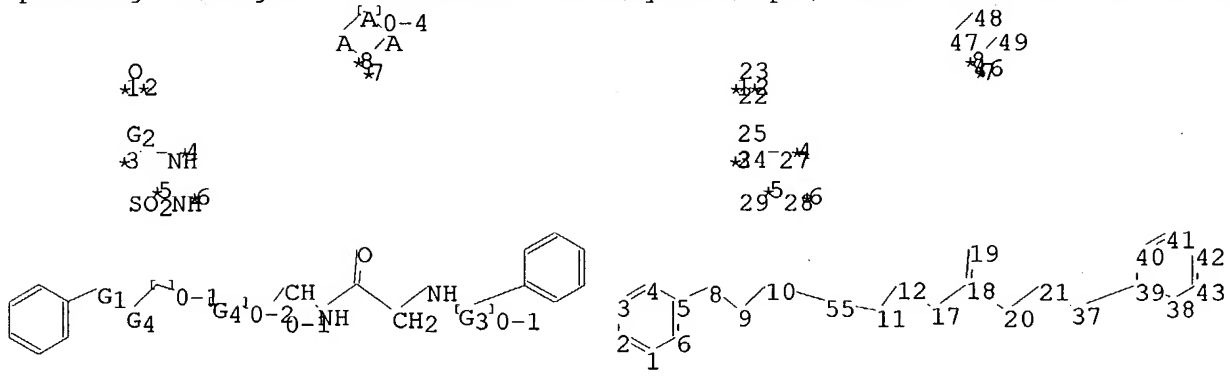
G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

```
G4:C,[*7-*8]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS



L10     STRUCTURE UPLOADED

=> que L10 AND L8 NOT L9

L11  QUE L10 AND L8 NOT L9

=> d l11
L11 HAS NO ANSWERS
L8              SCR 1839
L9              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L10             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L11             QUE  L10 AND L8 NOT L9


=> s l11 sss sam
SAMPLE SEARCH INITIATED 16:53:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  22600 TO ITERATE

  4.4% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       443011 TO   460989
PROJECTED ANSWERS:               0 TO        0

L12          0 SEA SSS SAM L10 AND L8 NOT L9

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L13   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L14   SCREEN CREATED
```

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 3).str



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49
chain bonds :
5-8 8-9 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 46-47
46-49 47-48 48-49
exact/norm bonds :
5-8 8-9 9-10 10-55 11-55 12-17 17-18 18-19 21-37 22-23 24-25 24-27
28-29 37-39 46-47 46-49 47-48 48-49
exact bonds :
11-12 18-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

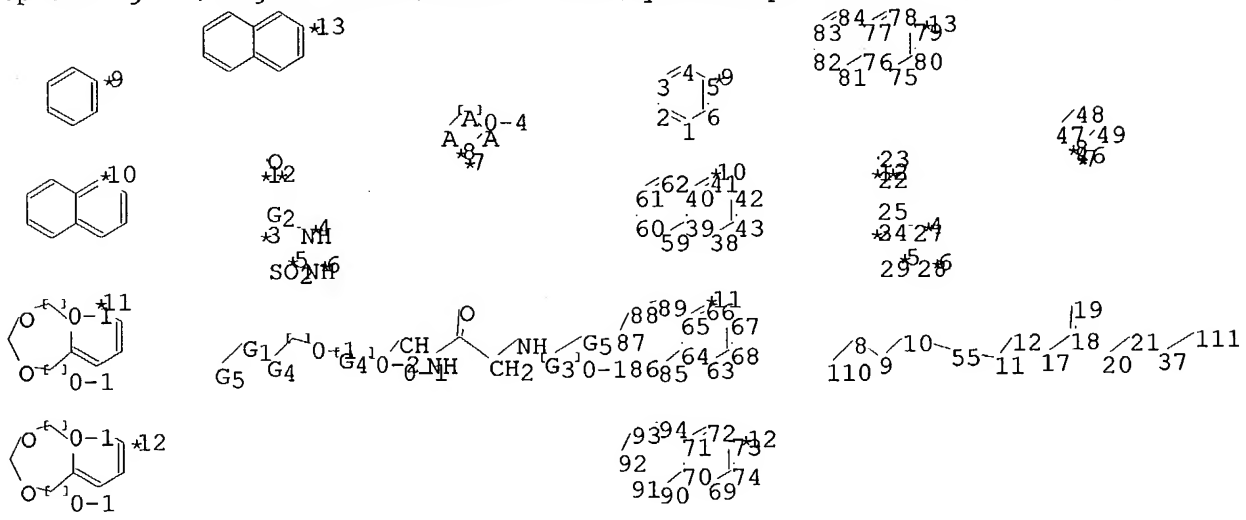
G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

```
G4:C,[*7-*8]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS



L15     STRUCTURE UPLOADED

=> que L15 AND L13 NOT L14

L16  QUE L15 AND L13 NOT L14

=> d l16
L16 HAS NO ANSWERS
L13             SCR 1839
L14             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L15             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L16             QUE  L15 AND L13 NOT L14


=> s l16 sss sam
SAMPLE SEARCH INITIATED 16:57:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  22600 TO ITERATE

  4.4% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       443011 TO   460989
PROJECTED ANSWERS:               0 TO        0

L17           0 SEA SSS SAM L15 AND L13 NOT L14

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L18   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L19   SCREEN CREATED
```

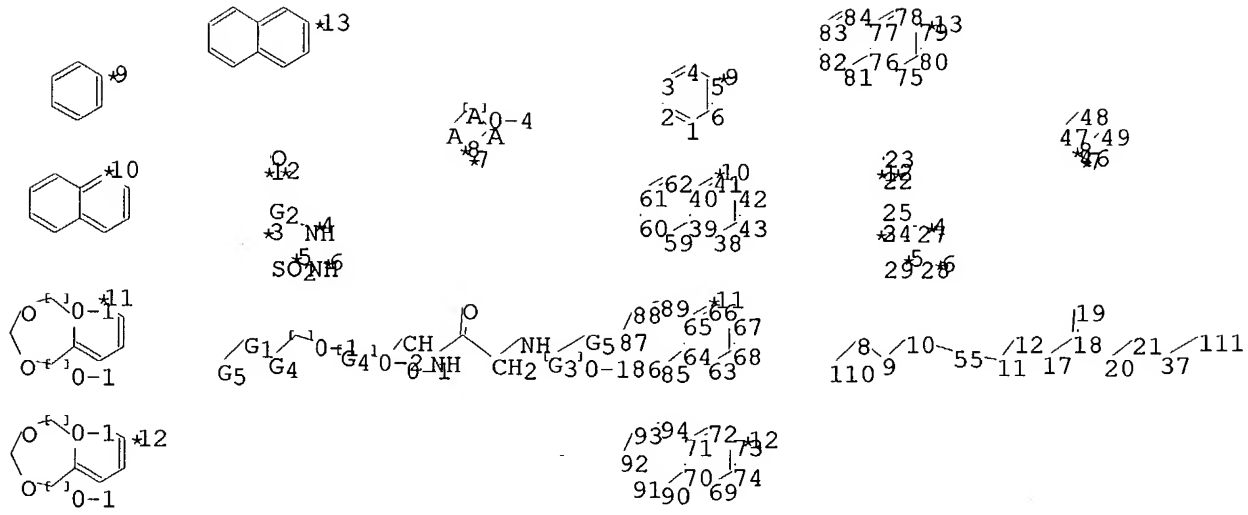
=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 4).str



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55 110 111
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85
86 87 88 89 90 91 92 93 94
chain bonds :
8-9 8-110 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-111
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-59 40-41 40-62 41-42
42-43 46-47 46-49 47-48 48-49 59-60 60-61 61-62 63-64 63-68 64-65 64-85
65-66 65-89 66-67 67-68 69-70 69-74 70-71 70-90 71-72 71-94 72-73 73-74
75-76 75-80 76-77 76-81 77-78 77-84 78-79 79-80 81-82 82-83 83-84 85-86
86-87 87-88 88-89 90-91 91-92 92-93 93-94

```
exact/norm bonds :
8-9  8-110  9-10  10-55  11-55  12-17  17-18  18-19  21-37  22-23  24-25  24-27
28-29  37-111  46-47  46-49  47-48  48-49
exact bonds :
11-12  18-20  20-21  64-85  65-89  70-90  71-94  85-86  86-87  87-88  88-89  90-91
91-92  92-93  93-94
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  38-39  38-43  39-40  39-59  40-41  40-62  41-42
42-43  59-60  60-61  61-62  63-64  63-68  64-65  65-66  66-67  67-68  69-70  69-74
70-71  71-72  72-73  73-74  75-76  75-80  76-77  76-81  77-78  77-84  78-79  79-80
81-82  82-83  83-84
isolated ring systems :
containing 1 : 38 : 63 : 69 : 75 :


G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:C,[*7-*8]

G5:[*9],[*10],[*11],[*12],[*13]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS  59:Atom  60:Atom  61:Atom  62:Atom  63:Atom  64:Atom  65:Atom  66:Atom
67:Atom  68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom  74:Atom  75:Atom
76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  81:Atom  82:Atom  83:Atom  84:Atom
85:Atom  86:Atom  87:Atom  88:Atom  89:Atom  90:Atom  91:Atom  92:Atom  93:Atom
94:Atom  110:CLASS  111:CLASS



L20     STRUCTURE UPLOADED

=> que L20 AND L18 NOT L19

L21  QUE L20 AND L18 NOT L19

=> d l21
L21 HAS NO ANSWERS
L18             SCR 1839
L19             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L20             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L21             QUE  L20 AND L18 NOT L19


=> s l21 sss sam
SAMPLE SEARCH INITIATED 17:06:00 FILE 'REGISTRY'
```

```
SAMPLE SCREEN SEARCH COMPLETED -  46361 TO ITERATE

  2.2% PROCESSED    1000 ITERATIONS                          1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       914391 TO   940049
PROJECTED ANSWERS:             519 TO     1335

L22           1 SEA SSS SAM L20 AND L18 NOT L19

=> => ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L23   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L24   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 5).str
```



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 55 110 111
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 46 47 48 49 59 60 61 62 63 64
65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85
86 87 88 89 90 91 92 93 94
chain bonds :
8-9 8-110 9-10 10-55 11-12 11-55 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-111
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-59 40-41 40-62 41-42
42-43 46-47 46-49 47-48 48-49 59-60 60-61 61-62 63-64 63-68 64-65 64-85
65-66 65-89 66-67 67-68 69-70 69-74 70-71 70-90 71-72 71-94 72-73 73-74
75-76 75-80 76-77 76-81 77-78 77-84 78-79 79-80 81-82 82-83 83-84 85-86
86-87 87-88 88-89 90-91 91-92 92-93 93-94

```
exact/norm bonds :
8-9  8-110  9-10  10-55  11-55  12-17  17-18  18-19  21-37  22-23  24-25  24-27
28-29  37-111  46-47  46-49  47-48  48-49
exact bonds :
11-12  18-20  20-21  64-85  65-89  70-90  71-94  85-86  86-87  87-88  88-89  90-91
91-92  92-93  93-94
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  38-39  38-43  39-40  39-59  40-41  40-62  41-42
42-43  59-60  60-61  61-62  63-64  63-68  64-65  65-66  66-67  67-68  69-70  69-74
70-71  71-72  72-73  73-74  75-76  75-80  76-77  76-81  77-78  77-84  78-79  79-80
81-82  82-83  83-84
isolated ring systems :
containing 1 : 38 : 63 : 69 : 75 :


G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:CH,[*7-*8]

G5:[*9],[*10],[*11],[*12],[*13]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  46:Atom  47:Atom  48:Atom  49:Atom
55:CLASS  59:Atom  60:Atom  61:Atom  62:Atom  63:Atom  64:Atom  65:Atom  66:Atom
67:Atom  68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom  74:Atom  75:Atom
76:Atom  77:Atom  78:Atom  79:Atom  80:Atom  81:Atom  82:Atom  83:Atom  84:Atom
85:Atom  86:Atom  87:Atom  88:Atom  89:Atom  90:Atom  91:Atom  92:Atom  93:Atom
94:Atom  110:CLASS  111:CLASS



L25     STRUCTURE UPLOADED

=> que L25 AND L23 NOT L24

L26  QUE L25 AND L23 NOT L24

=> d l26
L26 HAS NO ANSWERS
L23             SCR 1839
L24             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L25             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L26             QUE  L25 AND L23 NOT L24


=> s l26 sss sam
SAMPLE SEARCH INITIATED 17:08:34 FILE 'REGISTRY'
```

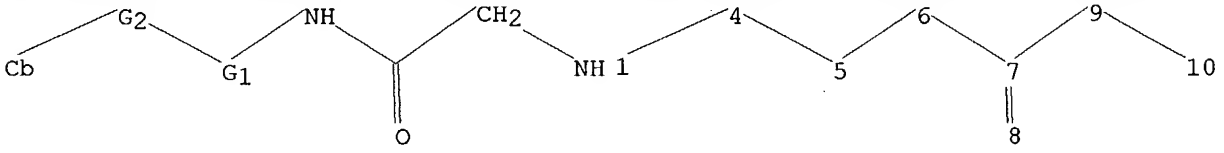
SAMPLE SCREEN SEARCH COMPLETED - 46361 TO ITERATE

2.2% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 914391 TO 940049
PROJECTED ANSWERS: 0 TO 0

L27 0 SEA SSS SAM L25 AND L23 NOT L24

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (genus).str



chain nodes :
1 4 5 6 7 8 9 10
chain bonds :
1-4 4-5 5-6 6-7 7-8 7-9 9-10
exact/norm bonds :
1-4 4-5 5-6 6-7 7-8
exact bonds :
7-9 9-10

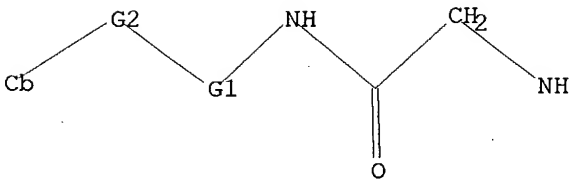
G1:Cy,Ak

G2:O,N

Match level :
1:Atom 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
Generic attributes :
1:
Saturation : Unsaturated

L28 STRUCTURE UPLOADED

=> d l28
L28 HAS NO ANSWERS
L28 STR



G1 Cy,Ak

G2 O,N

Structure attributes must be viewed using STN Express query preparation.

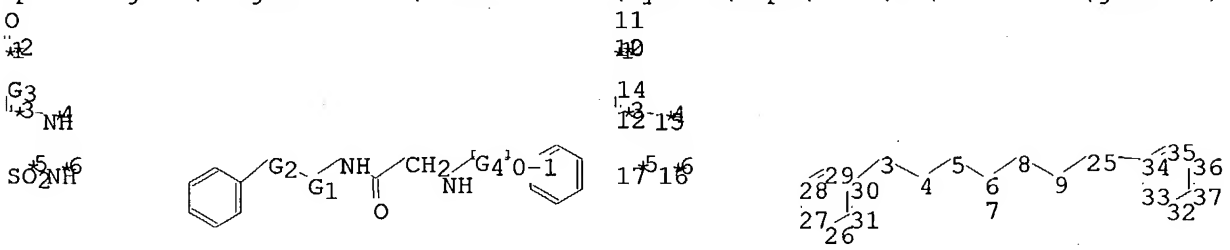
=> s l28 sss sam
SAMPLE SEARCH INITIATED 17:19:58 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 76144 TO ITERATE

1.3% PROCESSED 1000 ITERATIONS 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 5044

L29 4 SEA SSS SAM L28

=> =>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (genus 1).str



chain nodes :
3 4 5 6 7 8 9 10 11 12 14 15 16 17 25
ring nodes :
26 27 28 29 30 31 32 33 34 35 36 37
chain bonds :

```
3-4  3-30  4-5  5-6  6-7  6-8  8-9  9-25  10-11  12-14  12-15  16-17  25-34
ring bonds :
26-27  26-31  27-28  28-29  29-30  30-31  32-33  32-37  33-34  34-35  35-36  36-37
exact/norm bonds :
3-4  3-30  4-5  5-6  6-7  9-25  10-11  12-14  12-15  16-17  25-34
exact bonds :
6-8  8-9
normalized bonds :
26-27  26-31  27-28  28-29  29-30  30-31  32-33  32-37  33-34  34-35  35-36  36-37


G1:Cy,Ak

G2:O,N

G3:O,S

G4:SO2,[*1-*2],[*3-*4],[*5-*6]

Match level :
3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS  10:CLASS  11:CLASS
12:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  25:CLASS  26:Atom  27:Atom
28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom
37:Atom



L30     STRUCTURE UPLOADED

=> d l30
L30 HAS NO ANSWERS
L30             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l30 sss sam
SAMPLE SEARCH INITIATED 17:23:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  25618 TO ITERATE

  3.9% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       502794 TO   521926
PROJECTED ANSWERS:               0 TO        0

L31           0 SEA SSS SAM L30

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end
```

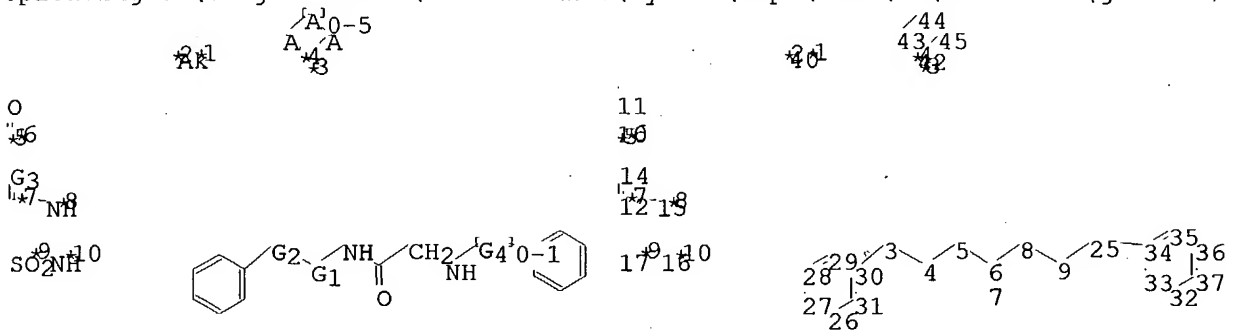
=> screen 1839

L32 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L33 SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (genus 2).str



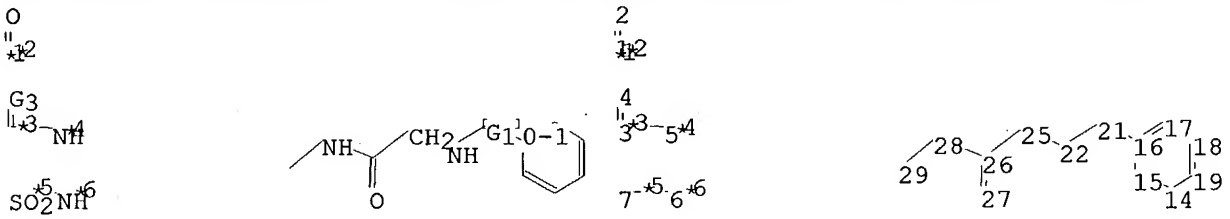
chain nodes :
3 4 5 6 7 8 9 10 11 12 14 15 16 17 25 40
ring nodes :
26 27 28 29 30 31 32 33 34 35 36 37 42 43 44 45
chain bonds :
3-4 3-30 4-5 5-6 6-7 6-8 8-9 9-25 10-11 12-14 12-15 16-17 25-34
ring bonds :
26-27 26-31 27-28 28-29 29-30 30-31 32-33 32-37 33-34 34-35 35-36 36-37
42-43 42-45 43-44 44-45
exact/norm bonds :
3-4 3-30 4-5 5-6 6-7 9-25 10-11 12-14 12-15 16-17 25-34 42-43 42-45
43-44 44-45
exact bonds :
6-8 8-9
normalized bonds :
26-27 26-31 27-28 28-29 29-30 30-31 32-33 32-37 33-34 34-35 35-36 36-37

G1:[*1-*2],[*3-*4]

```
G2:O,N

G3:O,S

G4:SO2,[*5-*6],[*7-*8],[*9-*10]

Connectivity :
40:3 X maximum RC ring/chain
Match level :
3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS  9:CLASS  10:CLASS  11:CLASS
12:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  25:CLASS  26:Atom  27:Atom
28:Atom  29:Atom  30:Atom  31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom
37:Atom  40:CLASS  42:Atom  43:Atom  44:Atom  45:Atom
Generic attributes :
40:
Saturation           : Saturated
Number of Carbon Atoms : less than 7

Element Count :
Node 40: Limited
    C,C1-4




L34     STRUCTURE UPLOADED

=> que L34 AND L32 NOT L33

L35  QUE L34 AND L32 NOT L33

=> d 135
L35 HAS NO ANSWERS
L32             SCR 1839
L33             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L34             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L35             QUE  L34 AND L32 NOT L33


=> s 135 sss sam
SAMPLE SEARCH INITIATED 17:28:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  24554 TO ITERATE

  4.1% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       481713 TO   500447
PROJECTED ANSWERS:               0 TO        0
```

L36 0 SEA SSS SAM L34 AND L32 NOT L33

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (broad).str



chain nodes :
1 2 3 4 5 6 7 21 22 25 26 27 28 29
ring nodes :
14 15 16 17 18 19
chain bonds :
1-2 3-4 3-5 6-7 16-21 21-22 22-25 25-26 26-27 26-28 28-29
ring bonds :
14-15 14-19 15-16 16-17 17-18 18-19
exact/norm bonds :
1-2 3-4 3-5 6-7 16-21 21-22 26-27 26-28 28-29
exact bonds :
22-25 25-26
normalized bonds :
14-15 14-19 15-16 16-17 17-18 18-19

G1:SO2,[*1-*2],[*3-*4],[*5-*6]

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 14:Atom 15:Atom
16:Atom 17:Atom 18:Atom 19:Atom 21:CLASS 22:CLASS 25:CLASS 26:CLASS
27:CLASS 28:CLASS 29:CLASS

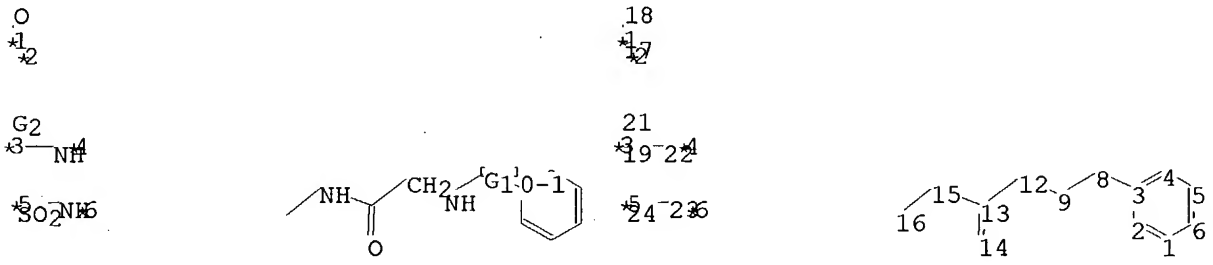
L37 STRUCTURE UPLOADED

=> d l37
L37 HAS NO ANSWERS
L37 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

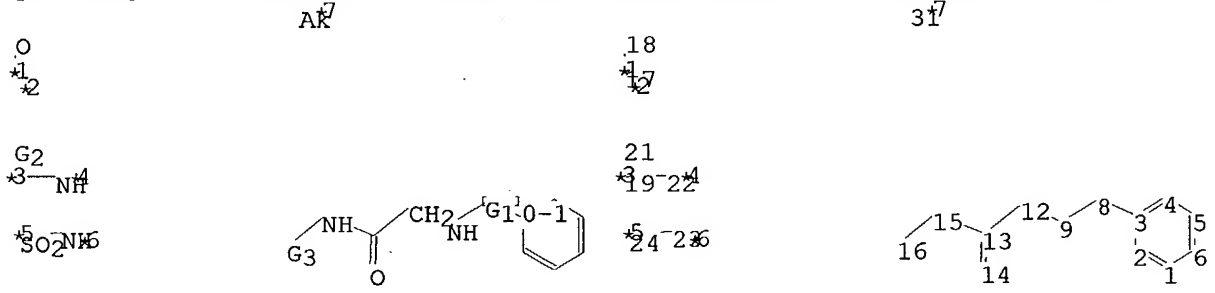
Structure attributes must be viewed using STN Express query preparation.

```
=> s l37 sss sam
SEARCH FAILED DUE TO A STRUCTURE QUERY ERROR
The structure query could not be searched.  Please review and revise
your structure query, especially checking the variable definitions and
attachments. In rare instances the failure may be due to a system
problem. Please contact your local STN Help Desk if you need
assistance.

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (broad 1).str
```



```
chain nodes :
8  9  12  13  14  15  16  17  18  19  21  22  23  24
ring nodes :
1  2  3  4  5  6
chain bonds :
3-8  8-9  9-12  12-13  13-14  13-15  15-16  17-18  19-21  19-22  23-24
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
3-8  8-9  13-14  13-15  15-16  17-18  19-21  19-22  23-24
exact bonds :
9-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


G1:SO2,[*1-*2],[*3-*4],[*5-*6]

G2:O,S

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  12:CLASS
13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS  19:CLASS  21:CLASS
22:CLASS  23:CLASS  24:CLASS
```

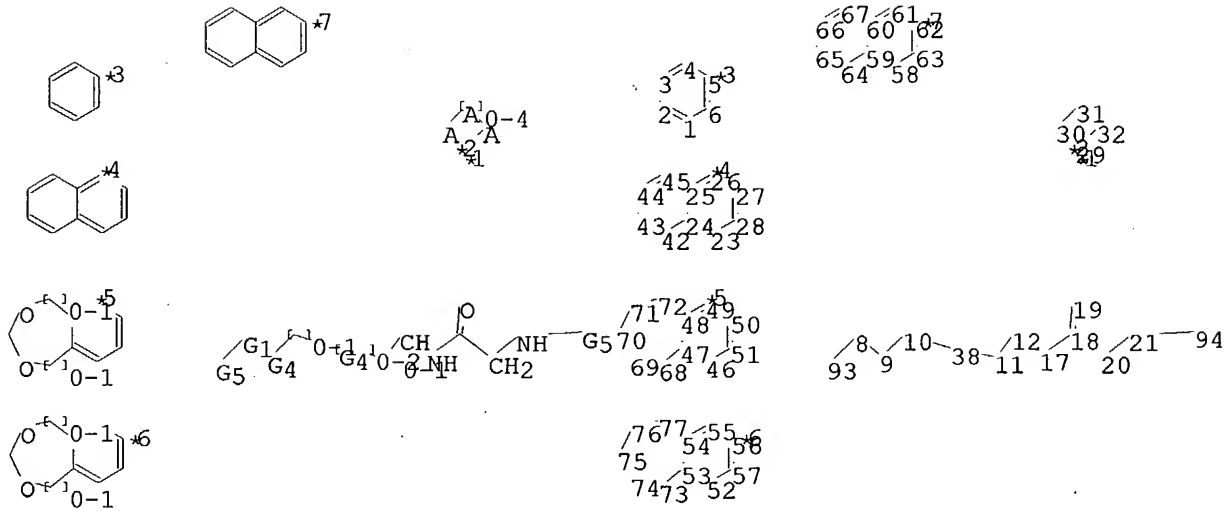
```
L38     STRUCTURE UPLOADED

=> d l38
L38 HAS NO ANSWERS
L38             STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s l38 sss sam
SAMPLE SEARCH INITIATED 17:34:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  70642 TO ITERATE

  1.4% PROCESSED    1000 ITERATIONS                                 2 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS    2112

L39           2 SEA SSS SAM L38

=> =>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (broad 2).str
```




```
chain nodes :
8  9  12  13  14  15  17  18  19  21  22  23  24  31
ring nodes :
```

```
1  2  3  4  5  6
ring/chain nodes :
16
chain bonds :
3-8  8-9  9-12  12-13  13-14  13-15  15-16  17-18  19-21  19-22  23-24
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
3-8  8-9  13-14  13-15  15-16  17-18  19-21  19-22  23-24
exact bonds :
9-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


G1:SO2,[*1-*2],[*3-*4],[*5-*6]

G2:O,S

G3:Cy,[*7]

Connectivity :
31:2 X maximum RC ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  12:CLASS
13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS  19:CLASS  21:CLASS
22:CLASS  23:CLASS  24:CLASS  31:CLASS
Generic attributes :
31:
Saturation              : Saturated
Number of Carbon Atoms : less than 7

Element Count :
Node 31: Limited
    C,C1-4




L40     STRUCTURE UPLOADED

=> d l40
L40 HAS NO ANSWERS
L40             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s l40 sss sam
SAMPLE SEARCH INITIATED 17:38:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  60423 TO ITERATE

  1.7% PROCESSED    1000 ITERATIONS                          1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
```

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:      EXCEEDS 1000000
PROJECTED ANSWERS:         EXCEEDS     742

L41           1 SEA SSS SAM L40

=> => ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L42   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L43   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 6).str
```



chain nodes :
8 9 10 11 12 17 18 19 20 21 38 93 94
ring nodes :
1 2 3 4 5 6 23 24 25 26 27 28 29 30 31 32 42 43 44 45 46 47
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68
69 70 71 72 73 74 75 76 77
chain bonds :
8-9 8-93 9-10 10-38 11-12 11-38 12-17 17-18 18-19 18-20 20-21 21-94
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 23-24 23-28 24-25 24-42 25-26 25-45 26-27
27-28 29-30 29-32 30-31 31-32 42-43 43-44 44-45 46-47 46-51 47-48 47-68
48-49 48-72 49-50 50-51 52-53 52-57 53-54 53-73 54-55 54-77 55-56 56-57
58-59 58-63 59-60 59-64 60-61 60-67 61-62 62-63 64-65 65-66 66-67 68-69
69-70 70-71 71-72 73-74 74-75 75-76 76-77
exact/norm bonds :

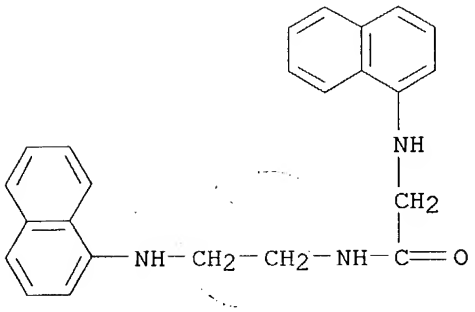
```
8-9  8-93  9-10  10-38  11-38  12-17  17-18  18-19  21-94  29-30  29-32  30-31
31-32
exact bonds :
11-12  18-20  20-21  47-68  48-72  53-73  54-77  68-69  69-70  70-71  71-72  73-74
74-75  75-76  76-77
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  23-24  23-28  24-25  24-42  25-26  25-45  26-27
27-28  42-43  43-44  44-45  46-47  46-51  47-48  48-49  49-50  50-51  52-53  52-57
53-54  54-55  55-56  56-57  58-59  58-63  59-60  59-64  60-61  60-67  61-62  62-63
64-65  65-66  66-67
isolated ring systems :
containing 1 : 23 : 46 : 52 : 58 :


G1:O,N

G2:O,S

G4:CH,[*1-*2]

G5:[*3],[*4],[*5],[*6],[*7]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  23:Atom
24:Atom  25:Atom  26:Atom  27:Atom  28:Atom  29:Atom  30:Atom  31:Atom  32:Atom
38:CLASS  42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:Atom  48:Atom  49:Atom
50:Atom  51:Atom  52:Atom  53:Atom  54:Atom  55:Atom  56:Atom  57:Atom  58:Atom
59:Atom  60:Atom  61:Atom  62:Atom  63:Atom  64:Atom  65:Atom  66:Atom  67:Atom
68:Atom  69:Atom  70:Atom  71:Atom  72:Atom  73:Atom  74:Atom  75:Atom  76:Atom
77:Atom  93:CLASS  94:CLASS



L44     STRUCTURE UPLOADED

=> que L44 AND L42 NOT L43

L45  QUE L44 AND L42 NOT L43

=> d l45
L45 HAS NO ANSWERS
L42             SCR 1839
L43             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L44             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L45             QUE  L44 AND L42 NOT L43


=> s l45 sss sam
SAMPLE SEARCH INITIATED 17:41:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2347 TO ITERATE

 42.6% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
```

```
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         44035 TO    49845
PROJECTED ANSWERS:                0 TO        0

L46           0 SEA SSS SAM L44 AND L42 NOT L43

=> s l45 sss ful
FULL SEARCH INITIATED 17:42:19 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  47892 TO ITERATE

100.0% PROCESSED   47892 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L47           3 SEA SSS FUL L44 AND L42 NOT L43

=> => s l47
L48           2 L47

=> d l47 1-2 bib,ab,hitstr
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:n


=> d l48 1-2 bib,ab,hitstr
```

L48 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:679833 CAPLUS
DN 115:279833
TI Preparation of bis[(quinolylamino)ethylamine and analogs as N-methyl-D-aspartic acid (NMDA) receptor antagonists
IN Antoku, Fujio; Saji, Ikutaro; Ohashi, Naohito; Nagata, Ryu
PA Sumitomo Pharmaceuticals Co., Ltd., Japan
SO Eur. Pat. Appl., 43 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

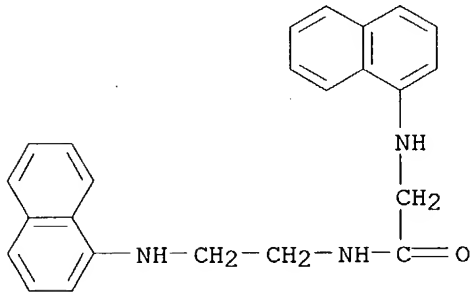
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 443862	A1	19910828	EP 1991-301417	19910222
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 04211040	A2	19920803	JP 1991-48974	19910220
	CA 2036781	AA	19910823	CA 1991-2036781	19910221
PRAI	JP 1990-43638		19900222		

OS MARPAT 115:279833
AB Ar1NR1A1NR2A2NR3Ar2 [I; Ar1 = (un)substituted aryl, 6-membered heterocyclyl containing 1-3 N, bicyclic heterocyclyl having a 5-membered hetero ring fused to a benzene ring, etc.; Ar2 = (un)substituted naphthyl, bicyclic heterocyclyl having a 5-membered hetero ring with 1-3 N atoms fused to a benzene ring, etc.; A1, A2 = (oxo-substituted) alkylene; R1-R3 = H, alkyl, aryl, arylalkyl, arylalkoxycarbonyl, alkylalkoxycarbonyl, acyl] and salts, useful in the prevention or treatment of symptoms associated with cerebral apoplexy or cerebral infarction, were prepared A stirred mixture of 8-aminoquinoline 0.1, HCl.NH(CH2CH2Cl)2 0.1, and Na2CO3 0.2 mol in 100 mL BuOH was refluxed for 35.5 h to give 3.9% title triamine which was converted to its HCl salt (II). II in mice inhibited NMDA-induced convulsions with ED50 = 16.4 mg/kg i.p., and in an in vitro competitive binding test with [3H]MK 801, II had IC50 of 1.3 μM. Approx. 22 I were prepared
IT **137582-78-6P 137582-79-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of methylaspartate receptor antagonist)
RN 137582-78-6 CAPLUS
CN Acetamide, 2-(1-naphthalenylamino)-N-[2-(1-naphthalenylamino)ethyl]-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

RN 137582-79-7 CAPLUS
CN Acetamide, 2-(1-naphthalenylamino)-N-[2-(1-naphthalenylamino)ethyl]- (9CI) (CA INDEX NAME)

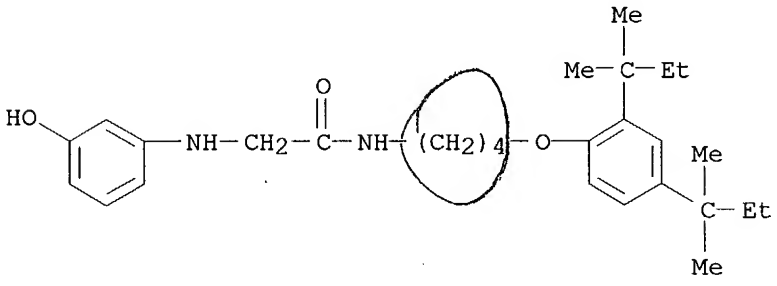


L48 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:22885 CAPLUS
DN 94:22885
TI Photosensitive silver halide photographic materials
IN Fujiwara, Mitsuto; Kaneko, Yutaka; Kawasaki, Mikio; Masukawa, Toyoaki; Matsuo, Shunji
PA Konishiroku Photo Industry Co., Ltd., Japan
SO U.S., 42 pp. Cont.-in-part of U.S. Ser. No. 726,635, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4200466	A	19800429	US 1978-874056	19780201
	JP 52042725	A2	19770402	JP 1975-118480	19750930
PRAI	JP 1975-118480		19750930		
	US 1976-726635		19760927		

AB Photog. materials which are capable of producing a neutral black dye image of excellent stability to oxidation without having to be subjected to a special image stabilization treatment contain a m-aminophenol derivative I (R,R2 = H, halo, or a split-off group or ≥1 is OH, SH, NH2, alkylamino, or arylamino and the other a H, halo, or a split-off group; R1,R3 = H, halo, OH, alkyl, alkoxy, alkylamido, arylamido, alkylsulfonamido, or arylsulfonamido; R4,R5 = H, alkyl, aralkyl, aryl, or alkenyl) as the black dye image forming coupler. These couplers are especially applicable to black-and-white photog. to produce imaging materials having a greatly reduced Ag content and greatly increased speed. Thus, II (prepared by treatment of m-aminophenol with N-dodecyl-β-bromoethylamide) 10 g was dissolved in EtOAc 30 mL and di-Bu phthalate 10 g, the solution mixed with 10% aqueous Alkanol B 5 mL and then dispersed in 5% aqueous gelatin 200 mL. This dispersion was added to a gelatin-Ag(Br,I) emulsion 500 g, and the emulsion coated on a cellulose triacetate support at 20 mg Ag/100 cm2 of support. The finished material was then exposed and developed to show a speed of 105, a γ of 0.46, a fog of 0.06, and a Dmax of 2.6 vs. 65, 0.22, 0.03, and 1.1, resp., for a II-free control and 100, 0.43, 0.05, and 2.7, resp., for a II-free control containing 40 mg Ag/100 cm2 of support.

IT **74935-58-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74935-58-3 CAPLUS
CN Acetamide, N-[4-[2,4-bis(1,1-dimethylpropyl)phenoxy]butyl]-2-[(3-hydroxyphenyl)amino]- (9CI) (CA INDEX NAME)



=> => ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end

=> screen 1839

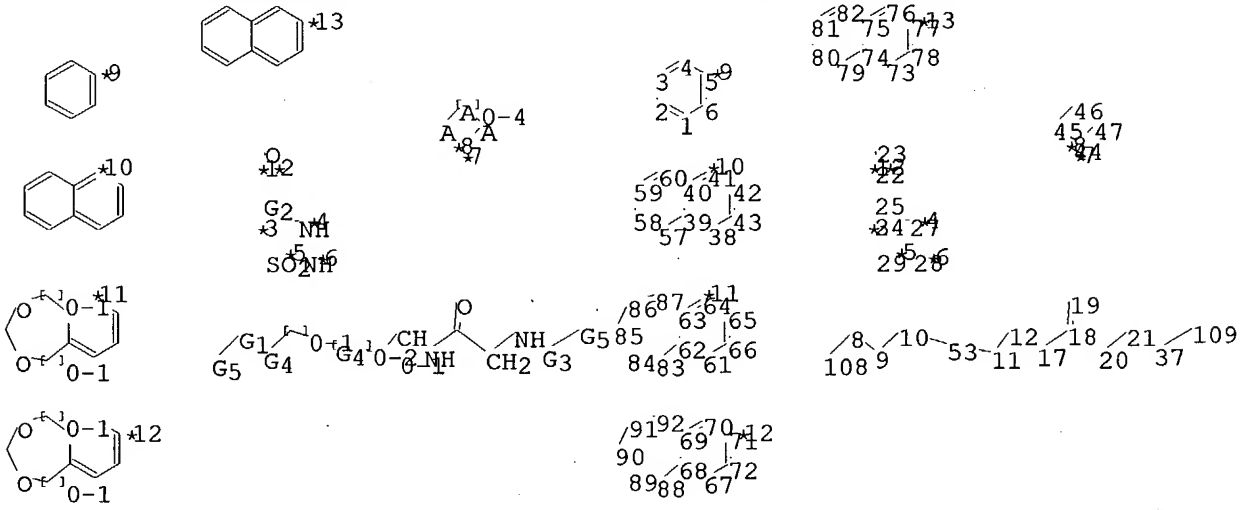
L49 SCREEN CREATED

=> screen 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047

L50 SCREEN CREATED

=>

Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 7).str



chain nodes :

8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53 108 109
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47 57 58 59 60 61 62
63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83
84 85 86 87 88 89 90 91 92
chain bonds :
8-9 8-108 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-109
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-57 40-41 40-60 41-42
42-43 44-45 44-47 45-46 46-47 57-58 58-59 59-60 61-62 61-66 62-63 62-83
63-64 63-87 64-65 65-66 67-68 67-72 68-69 68-88 69-70 69-92 70-71 71-72
73-74 73-78 74-75 74-79 75-76 75-82 76-77 77-78 79-80 80-81 81-82 83-84
84-85 85-86 86-87 88-89 89-90 90-91 91-92
exact/norm bonds :
8-9 8-108 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27
28-29 37-109 44-45 44-47 45-46 46-47
exact bonds :
11-12 18-20 20-21 62-83 63-87 68-88 69-92 83-84 84-85 85-86 86-87 88-89
89-90 90-91 91-92
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 39-57 40-41 40-60 41-42
42-43 57-58 58-59 59-60 61-62 61-66 62-63 63-64 64-65 65-66 67-68 67-72
68-69 69-70 70-71 71-72 73-74 73-78 74-75 74-79 75-76 75-82 76-77 77-78
79-80 80-81 81-82
isolated ring systems :
containing 1 : 38 : 61 : 67 : 73 :

G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:CH,[*7-*8]

G5:[*9],[*10],[*11],[*12],[*13]

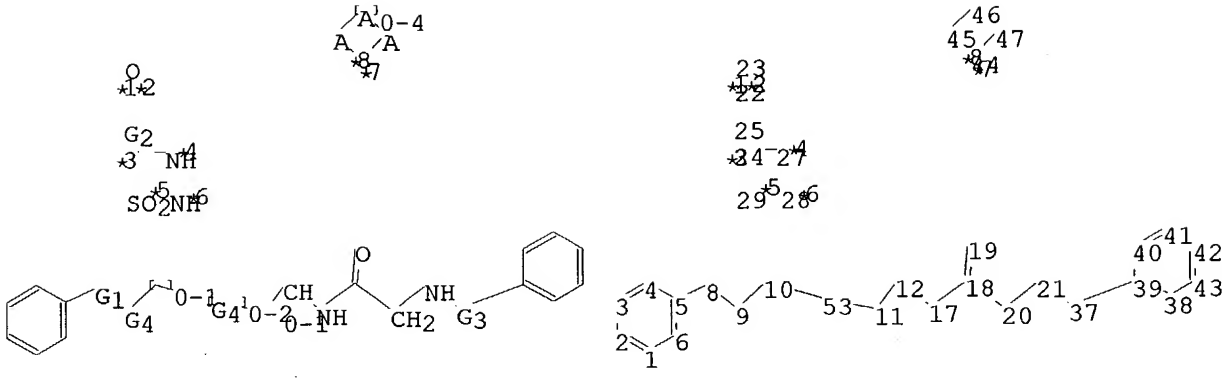
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 37:CLASS 38:Atom
39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom
53:CLASS 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom
65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom
74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom
83:Atom 84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 91:Atom
92:Atom 108:CLASS 109:CLASS

L51 STRUCTURE UPLOADED

=> que L51 AND L49 NOT L50

L52 QUE L51 AND L49 NOT L50

```
=> d l52
L52 HAS NO ANSWERS
L49             SCR 1839
L50             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L51             STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.
L52             QUE  L51 AND L49 NOT L50


=> s l52 sss sam
SAMPLE SEARCH INITIATED 17:46:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  36983 TO ITERATE

  2.7% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:       728186 TO   751134
PROJECTED ANSWERS:               0 TO        0

L53           0 SEA SSS SAM L51 AND L49 NOT L50

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L54   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L55   SCREEN CREATED

=>
Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 8).str
```



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47
chain bonds :
5-8 8-9 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 44-45
44-47 45-46 46-47
exact/norm bonds :
5-8 8-9 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27
28-29 37-39 44-45 44-47 45-46 46-47
exact bonds :
11-12 18-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

G1:O,N

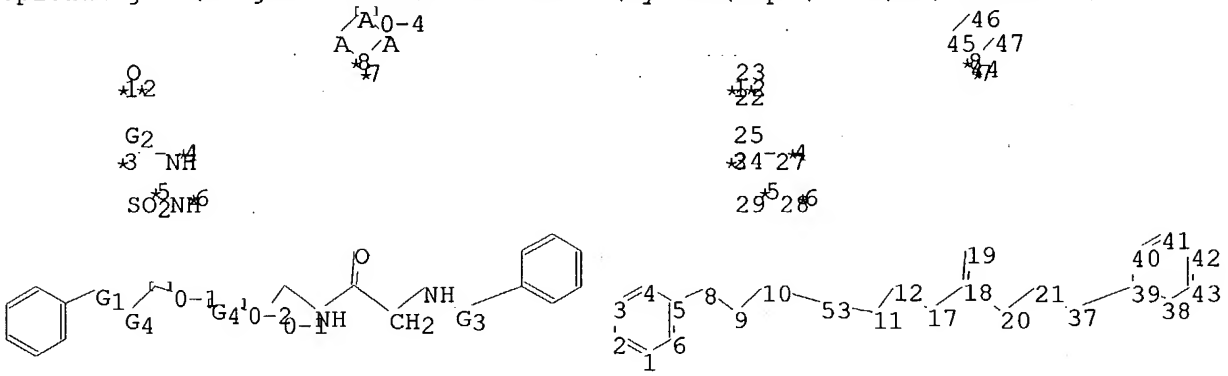
G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:C,[*7-*8]

```
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:Atom
53:CLASS



L56     STRUCTURE UPLOADED

=> que L56 AND L54 NOT L55

L57  QUE L56 AND L54 NOT L55

=> d l57
L57 HAS NO ANSWERS
L54             SCR 1839
L55             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L56             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L57             QUE  L56 AND L54 NOT L55


=> s l57 sss sam
SAMPLE SEARCH INITIATED 17:48:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   9195 TO ITERATE

 10.9% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       178155 TO   189645
PROJECTED ANSWERS:               0 TO        0

L58           0 SEA SSS SAM L56 AND L54 NOT L55

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L59   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L60   SCREEN CREATED

=>
```

Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 9).str



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47
chain bonds :
5-8 8-9 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 44-45
44-47 45-46 46-47
exact/norm bonds :
5-8 8-9 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27
28-29 37-39 44-45 44-47 45-46 46-47
exact bonds :
11-12 18-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

G1:O,N

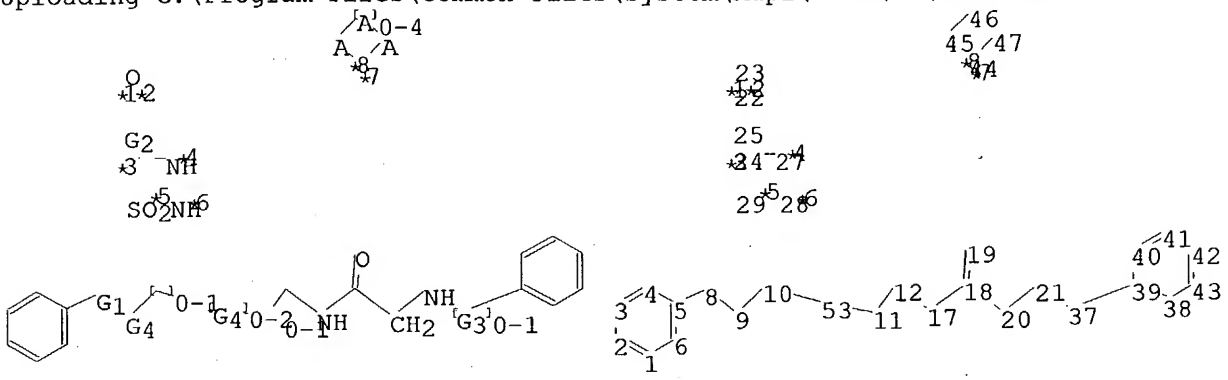
G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:C,[*7-*8]

```
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:Atom
53:CLASS



L61     STRUCTURE UPLOADED

=> que L61 AND L59 NOT L60

L62  QUE L61 AND L59 NOT L60

=> d l62
L62 HAS NO ANSWERS
L59             SCR 1839
L60             SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L61             STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L62             QUE  L61 AND L59 NOT L60


=> s l62 sss sam
SAMPLE SEARCH INITIATED 17:50:14 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   9195 TO ITERATE

 10.9% PROCESSED    1000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       178155 TO   189645
PROJECTED ANSWERS:               0 TO        0

L63           0 SEA SSS SAM L61 AND L59 NOT L60

=> ....Testing the current file.... screen

ENTER SCREEN EXPRESSION OR (END):end


=> screen 1839

L64   SCREEN CREATED

=> screen 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047

L65   SCREEN CREATED

=>
```

Uploading C:\Program Files\Common Files\System\Mapi\1033\NT\10027505 (rce 10).str



chain nodes :
8 9 10 11 12 17 18 19 20 21 22 23 24 25 27 28 29 37 53
ring nodes :
1 2 3 4 5 6 38 39 40 41 42 43 44 45 46 47
chain bonds :
5-8 8-9 9-10 10-53 11-12 11-53 12-17 17-18 18-19 18-20 20-21 21-37
22-23 24-25 24-27 28-29 37-39
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43 44-45
44-47 45-46 46-47
exact/norm bonds :
5-8 8-9 9-10 10-53 11-53 12-17 17-18 18-19 21-37 22-23 24-25 24-27
28-29 37-39 44-45 44-47 45-46 46-47
exact bonds :
11-12 18-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 38-39 38-43 39-40 40-41 41-42 42-43

G1:O,N

G2:O,S

G3:SO2,[*1-*2],[*3-*4],[*5-*6]

G4:C,[*7-*8]

```
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  8:CLASS  9:CLASS  10:CLASS
11:CLASS  12:CLASS  17:CLASS  18:CLASS  19:CLASS  20:CLASS  21:CLASS  22:CLASS
23:CLASS  24:CLASS  25:CLASS  27:CLASS  28:CLASS  29:CLASS  37:CLASS  38:Atom
39:Atom  40:Atom  41:Atom  42:Atom  43:Atom  44:Atom  45:Atom  46:Atom  47:Atom
53:CLASS



L66      STRUCTURE UPLOADED

=> que L66 AND L64 NOT L65

L67  QUE L66 AND L64 NOT L65

=> d l67
L67 HAS NO ANSWERS
L64              SCR 1839
L65              SCR 2016 OR 2026 OR 2039 OR 2040 OR 2045 OR 2047
L66              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L67              QUE  L66 AND L64 NOT L65


=> s l67 sss sam
SAMPLE SEARCH INITIATED 17:51:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  22600 TO ITERATE

  4.4% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       443011 TO   460989
PROJECTED ANSWERS:               0 TO        0

L68           0 SEA SSS SAM L66 AND L64 NOT L65

=> s l62 sss sam
SAMPLE SEARCH INITIATED 17:52:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   9195 TO ITERATE

 10.9% PROCESSED    1000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       178155 TO   189645
PROJECTED ANSWERS:               0 TO        0

L69           0 SEA SSS SAM L61 AND L59 NOT L60
```

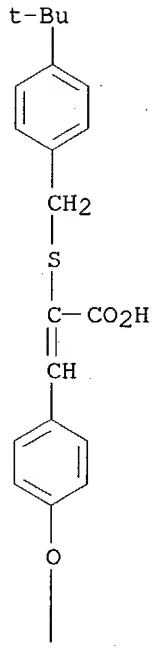
```
=> s l62 sss ful
FULL SEARCH INITIATED 17:52:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 183719 TO ITERATE

100.0% PROCESSED  183719 ITERATIONS                          67 ANSWERS
SEARCH TIME: 00.00.03

L70           67 SEA SSS FUL L61 AND L59 NOT L60

=> => s l70
L71           47 L70

=> d l71 1-47 bib,ab,hitstr
```

L71 ANSWER 1 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:271704 CAPLUS
DN 138:304056
TI Preparation of 2-phenylalkylthio-3-phenyl-2-propenoic acids and Cdc25 phosphatase inhibitors
IN Kitaide, Makoto; Nagai, Kentaro; Terada, Tadashi; Asao, Tetsuji; Sugimoto, Yoshikazu; Yamada, Yuji
PA Taiho Pharmaceutical Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 24 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

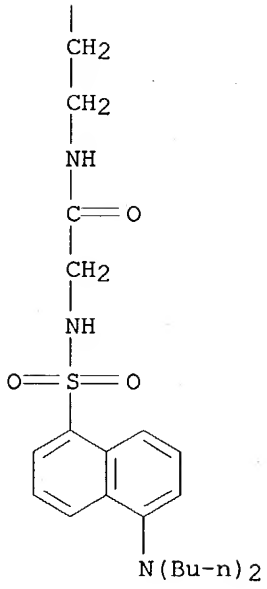
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2003104964	A2	20030409	JP 2001-301335	20010928
PRAI JP 2001-301335		20010928		

OS MARPAT 138:304056
AB The compds. I [R1 = H, cycloalkyl, Ph, naphthyl, pyridyl, phenylpyrazolyl, etc.; W = CH, N; X = O, OCH2, NR4; R4 = H, lower alkyl, (un)substituted aralkyl; Y = 1,4-piperazinyl, NHCHR5CONH, NH; R5 = H, (un)substituted lower alkyl; Z = CO2H, SO3H; R2 = alkyl, Ph, NR6R7; R6, R7 = lower alkyl; R3 = H, lower alkyl; j, k, n = 0, 1; l = 0-6; m = 1-10] or their pharmaceutically acceptable salts are prepared Me 3-[4-[(4-tert-butylphenyl)methoxy]phenyl]-2-[(4-tert-butylphenyl)methylthio]-2-propenoate was treated with NaOH in THF-MeOH at room temperature for 17 h to give 320 mg 2-[[4-tert-butylphenyl]methylthio]-3-[4-[(4-tert-butylphenyl)methoxy]phenyl]-2-propenoic acid showing Cdc25 phosphatase inhibitory activity IC50 of 3.6 μm.
IT **508180-73-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylalkylthiophenylpropenoic acids and Cdc25 phosphatase inhibitors)
RN 508180-73-2 CAPLUS
CN 2-Propenoic acid, 3-[4-[2-[[[[[5-(dibutylamino)-1-naphthalenyl]sulfonyl]amino]acetyl]amino]ethoxy]phenyl]-2-[[[4-(1,1-dimethylethyl)phenyl]methyl]thio]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

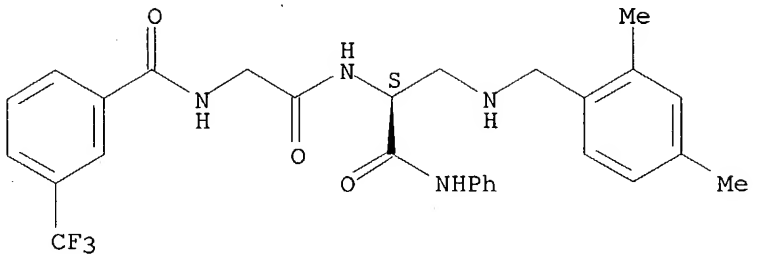


L71 ANSWER 2 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:487516 CAPLUS
DN 137:63474
TI Preparation of amino acid-related diamines as modulators of chemokine receptor activity
IN Carter, Percy; Cherney, Robert
PA Bristol-Myers Squibb Pharma Company, USA
SO PCT Int. Appl., 375 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002050019	A2	20020627	WO 2001-US50619	20011220
	WO 2002050019	A3	20030313		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2002041724	A5	20020701	AU 2002-41724	20011220
	US 2003060459	A1	20030327	US 2001-27505	20011220
	EP 1351924	A2	20031015	EP 2001-988415	20011220
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
PRAI	US 2000-256855P	P	20001220		
	WO 2001-US50619	W	20011220		

OS MARPAT 137:63474
AB Diamine compds. R1-X-CR6R7(CR8R9)m(CR10R11)lCR12R3NHCO(CR14R14a)nNR15-Z-R2 [Z = a bond, CONH, C(S)NH, SO2, SO2NH; X = NH, (cyclo)alkylimino, O, S, methyleneimino optionally substituted by (cyclo)alkyl; R1, R2 = (hetero)aryl; R3 = H, functionalized alkyl, (hetero)cyclyl; R6-R12 = alkyl, alkenyl, alkynyl, any group given for R3; R14, R14a = (un)substituted alkyl; n = 1 or 2; l, m = 0 or 1] or their pharmaceutically acceptable salt were prepared as modulators of chemokine receptor activity for use in the treatment and prevention of asthma, multiple sclerosis, atherosclerosis, and rheumatoid arthritis. One hundred ninety-four diamines, e.g., Me (2S)-3-[[(2,4-dimethylphenyl)methyl]amino]-2-[[[[3-(trifluoromethyl)benzoyl]amino]acetyl]amino]propanoate, were synthesized and claimed. All examples of the present invention have activity (IC50 = 50% at .ltorsim. 20 μM) in the antagonism of MCP-1 binding to human PBMC (human peripheral blood mononuclear cells).
IT **439148-73-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid-related diamines as modulators of chemokine receptor activity)
RN 439148-73-9 CAPLUS
CN L-Alaninamide, N-[3-(trifluoromethyl)benzoyl]glycyl-3-[[(2,4-dimethylphenyl)methyl]amino]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L71 ANSWER 3 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:275953 CAPLUS
DN 136:309851
TI Preparation of diphenylamines and N-nitrosodiphenylamines for treatment of oxidative stress and unavailability of endothelial nitric oxide.
IN Lardy, Claude; Nioche, Jean-Yves; Caputo, Lidia; Decerprit, Jacques; Ortholand, Jean-Yves; Festal, Didier; Guerrier, Daniel
PA Merck Patent G.m.b.H., Germany
SO PCT Int. Appl., 142 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002028820	A1	20020411	WO 2001-EP10761	20010918
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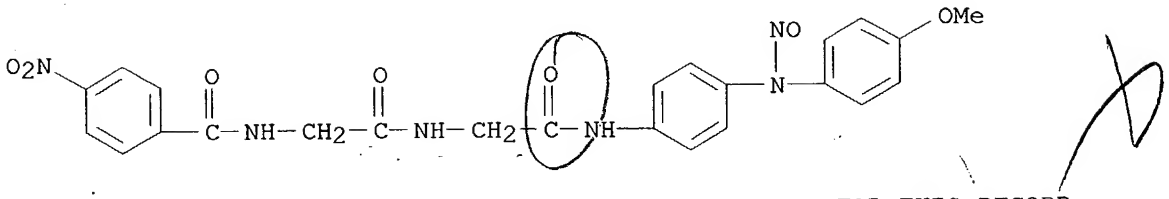
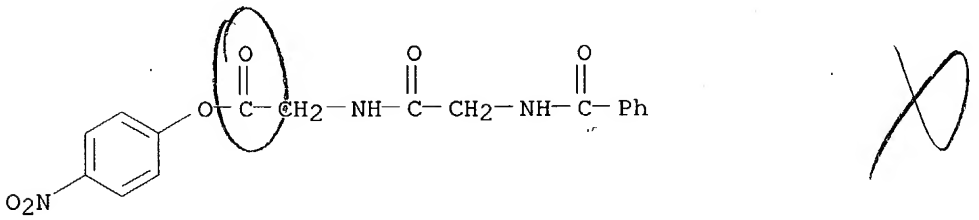
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	FR 2815030	A1	20020412	FR 2000-12749	20001005
	AU 2001089891	A5	20020415	AU 2001-89891	20010918
	BR 2001014252	A	20030701	BR 2001-14252	20010918
	EP 1322598	A1	20030702	EP 2001-969732	20010918
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	US 2004063783	A1	20040401	US 2003-398238	20030403
	NO 2003001533	A	20030404	NO 2003-1533	20030404
PRAI	FR 2000-12749	A	20001005		
	WO 2001-EP10761	W	20010918		

OS MARPAT 136:309851
AB Title compds. [I; X, Ra = H, (unsatd.) aliphatyl, AY; A = CO, SO2, CONRa, CONRaSO2; T = H, halo, NO2, cyano, (unsatd.) (halogenated) aliphatyl optionally interrupted by O and/or S; Y = organic substituent; with provisos], and des-nitroso compds. (II; variables as above), were prepared Thus, a mixture of nicotinoyl chloride hydrochloride, 4-amino-4'-methoxy-N-tert-butoxycarbonyldiphenylamine, and Et3N was stirred in CH2Cl2 to give 100% 4-nicotinoylamino derivative which was N-deprotected with CF3CO2H to give 95.2% 4-methoxy-4'-nicotinoylaminodiphenylamine. The latter in HOAc was treated dropwise with aqueous NaNO2 to give 88% N-nitroso-4-methoxy-4'-nicotinoylaminodiphenylamine. Tested II inhibited oxidation of human low mol. weight lipoproteins by Cu2+ with IC50 = 1.7-13.4 μM.
IT **409353-72-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diphenylamines and N-nitrosodiphenylamines for treatment of oxidative stress and unavailability of endothelial nitric oxide)
RN 409353-72-6 CAPLUS
CN Glycinamide, N-(4-nitrobenzoyl)glycyl-N-[4-[(4-methoxyphenyl)nitrosoamino]phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

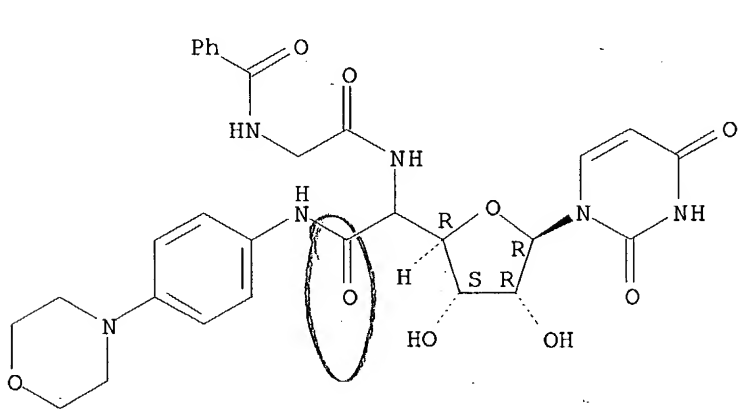
L71 ANSWER 4 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:752347 CAPLUS
DN 136:33788
TI Kinetic Evaluation of a Metalated Diglycine Conjugate as a Functional Mimetic of Phosphate Ester Hydrolase
AU Madhavaiah, C.; Verma, Sandeep
CS Department of Chemistry, Indian Institute of Technology-Kanpur, Kanpur (UP), 208016, India
SO Bioconjugate Chemistry (2001), 12(6), 855-860
CODEN: BCCHES; ISSN: 1043-1802
PB American Chemical Society
DT Journal
LA English
AB The crucial role of phosphate ester hydrolysis in various biol. processes has spurred vigorous research activities to understand mechanisms of phosphate ester hydrolysis and to develop model systems that assist the above-mentioned reaction in a catalytic fashion. In the present study, we describe a novel, metalated peptide conjugate 4 possessing phosphate ester hydrolyzing activity against a phosphate monoester, diester, and a RNA chemical model. The design of conjugate 4 is inspired by the ATCUN binding tripeptide motif of serum albumin and involves tethering of two diglycine units by a flexible 1,3-diaminopropane linker. Detailed kinetic investigations of phosphate ester hydrolysis using model substrates and efforts to decipher underlying mechanisms are presented.
IT **380365-66-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(kinetic evaluation of copper-metalated diglycine conjugate as a functional mimetic of phosphate ester hydrolase)
RN 380365-66-2 CAPLUS
CN Glycine, N-benzoylglycyl-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

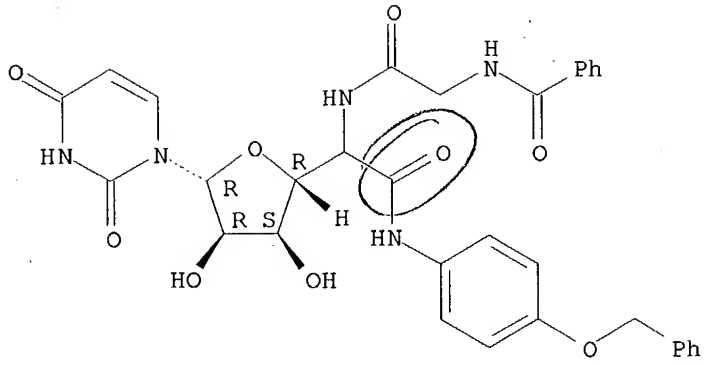
L71 ANSWER 5 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:430537 CAPLUS
DN 135:195737
TI Combinatorial synthesis of nikkomycin analogues on solid support
AU Suda, Atsushi; Ohta, Atsunori; Sudoh, Masayuki; Tsukuda, Takuo; Shimma, Nobuo
CS Combinatorial Chemistry Group, Department of Chemistry, Nippon Roche Research Center, Kanagawa, 247-8530, Japan
SO Heterocycles (2001), 55(6), 1023-1028
CODEN: HTCYAM; ISSN: 0385-5414
PB Japan Institute of Heterocyclic Chemistry
DT Journal
LA English
OS CASREACT 135:195737
AB Using Rink amide resin as the amine portion, a group of fifty-nine carboxylic acids, fifteen isocyanides, and 5'-deoxy-2',3'-O-(1-methylethylidene)-5'-oxo-uridine, generated in two steps from uridine, a four-component Ugi reaction was used to prepare a library of title compds., of which three proved to be as potent as nikkomycin Z as inhibitors of Candida albicans chitin synthase 1; only one showed inhibitory activity against C. albicans chitin synthase 2.
IT **356533-75-0P 356533-76-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of nikkomycin analog library on solid support using 4-component Ugi reaction)
RN 356533-75-0 CAPLUS
CN β-D-ribo-Hexopyranuronamide, 5-[[(benzoylamino)acetyl]amino]-1,5-dideoxy-1-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[4-(4-morpholinyl)phenyl]-, (5ξ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 356533-76-1 CAPLUS
CN β-D-ribo-Hexopyranuronamide, 5-[[(benzoylamino)acetyl]amino]-1,5-dideoxy-1-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-N-[4-(phenylmethoxy)phenyl]-, (5ξ)- (9CI) (CA INDEX NAME)

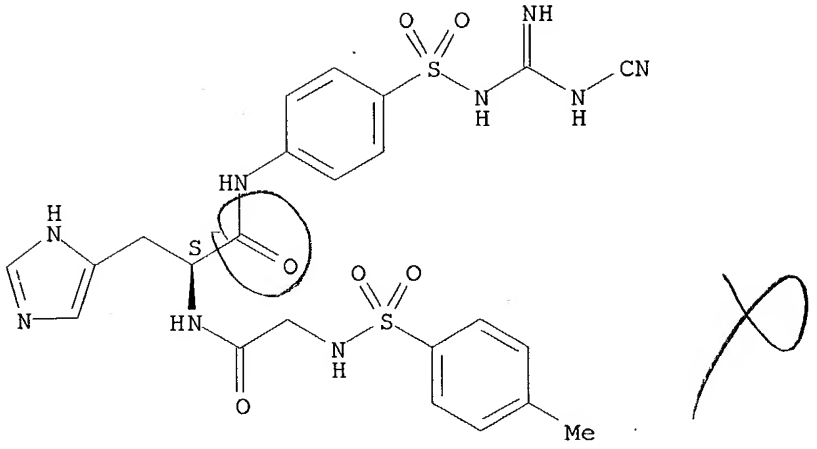
Absolute stereochemistry.



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

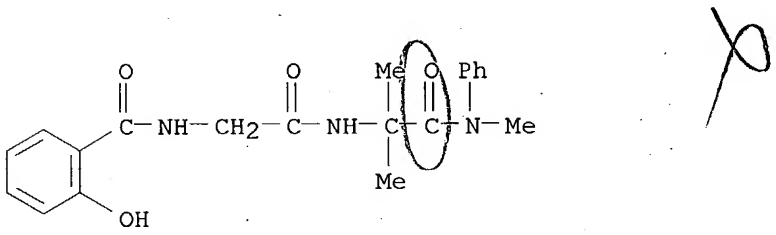
L71 ANSWER 6 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:271407 CAPLUS
DN 135:57729
TI Protease inhibitors, part 13: specific, weakly basic thrombin inhibitors incorporating sulfonyl dicyandiamide moieties in their structure
AU Clare, Brian W.; Scozzafava, Andrea; Supuran, Claudiu T.
CS Department of Chemistry, The University of Western Australia, Nedlands, 6009, Australia
SO Journal of Enzyme Inhibition (2001), 16(1), 1-13
CODEN: ENINEG; ISSN: 8755-5093
PB Harwood Academic Publishers
DT Journal
LA English
AB A series of compds. has been prepared by reaction of dicyandiamide with alkyl/arylsulfonyl halides as well as arylsulfonyl isocyanates to locate a lead for obtaining weakly basic thrombin inhibitors with sulfonyl dicyandiamide moieties as the S1 anchoring group. The detected lead was sulfanilyl-dicyandiamide (KI of 3 μM against thrombin, and 15 μM against trypsin), which has been further derivatized at the 4-amino group by incorporating arylsulfonylureido as well as amino acyl/dipeptidyl groups protected at the amino terminal moiety with benzyloxycarbonyl or tosylureido moieties. The best compound obtained (ts-D-Phe-Pro-sulfanilyl-dicyandiamide) showed inhibition consts. of 9 nM against thrombin and 1400 nM against trypsin. The pKa measurements showed that the new derivs. reported here do indeed possess a reduced basicity, with the pKa of the modified guanidine moieties in the range 7.9-8.3 pKa units. Mol. mechanics calcns. showed that the preferred tautomeric form of these compds. is of the type ArSO2N=C(NH2) NH-CN, probably allowing for the formation of favorable interaction between this new anchoring group and the active site amino acid residue Asp 189, critical for substrate/inhibitor binding to this type of serine protease. Thus, the main finding of the present paper is that the sulfonyldicyandiamide group may constitute an interesting alternative for obtaining weakly basic, potent thrombin inhibitors, which bind with less affinity to trypsin.
IT **345916-26-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of specific, weakly basic thrombin inhibitors incorporating sulfonyl dicyandiamide moieties in their structure)
RN 345916-26-9 CAPLUS
CN L-Histidinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[4-[[[(cyanoamino)iminomethyl]amino]sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L71 ANSWER 7 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:366202 CAPLUS
DN 127:95604
TI Synthesis of cyclic depsipeptides and peptides via direct amide cyclization
AU Villalgordo, Jose M.; Heimgartner, Heinz
CS Organisch-Chemisches Inst., Universitat Zurich, Zurich, CH-8057, Switz.
SO Helvetica Chimica Acta (1997), 80(3), 748-766
CODEN: HCACAV; ISSN: 0018-019X
PB Verlag Helvetica Chimica Acta
DT Journal
LA English
OS CASREACT 127:95604
AB The 2H-azirin-3-amines I [R = Me, R2 = (CH2)4] were used as amino acid synthons in the preparation of medium-sized cyclic depsipeptides and peptides derived from salicylates and anthranilic acid, resp. The combination of the "azirine/oxazolone method" for the synthesis of linear peptides containing α,α-disubstituted α-amino acids and the acid-catalyzed amide cyclization in DMF at 60° proved to be an excellent preparative route to 10-membered cyclic depsipeptides and peptides. In the case of the anthranilic acid derivative, a transannular ring-closure reaction was observed Larger rings proved to be extremely sensitive to hydrolysis.
IT **192046-51-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cyclic depsipeptides and peptides via direct amide cyclization)
RN 192046-51-8 CAPLUS
CN Alaninamide, N-(2-hydroxybenzoyl)glycyl-N,2-dimethyl-N-phenyl- (9CI) (CA INDEX NAME)



L71 ANSWER 8 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:290093 CAPLUS
DN 126:264011
TI Preparation of meta-guanidine, urea, thiourea or azacyclic amino benzoic acid derivatives as integrin antagonists
IN Ruminski, Peter Gerrard; Clare, Michael; Collins, Paul Waddell; Desai, Bipinchandra Nanubhai; Lindmark, Richard John; Rico, Joseph Gerace; Rogers, Thomas Edward; Russell, Mark Andrew; et al.
PA G.D. Searle and Co., USA; Ruminski, Peter Gerrard; Clare, Michael; Collins, Paul Waddell; Desai, Bipinchandra Nanubhai; Lindmark, Richard, John
SO PCT Int. Appl., 930 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9708145	A1	19970306	WO 1996-US13500	19960827
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM				
	CA 2230209	AA	19970306	CA 1996-2230209	19960827
	AU 9671039	A1	19970319	AU 1996-71039	19960827
	AU 702487	B2	19990225		
	EP 850221	A1	19980701	EP 1996-932142	19960827
	EP 850221	B1	20010718		
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	CN 1201454	A	19981209	CN 1996-197911	19960827
	CN 1085980	B	20020605		
	BR 9610422	A	19990713	BR 1996-10422	19960827
	JP 11510814	T2	19990921	JP 1996-510397	19960827
	IL 123164	A1	20010319	IL 1996-123164	19960827
	AT 203234	E	20010815	AT 1996-932142	19960827
	ES 2161373	T3	20011201	ES 1996-932142	19960827
	RU 2196769	C2	20030120	RU 1998-105408	19960827
	RO 118290	B1	20030430	RO 2001-1069	19960827
	RO 118289	B1	20030430	RO 1998-500	19960827
	PL 186370	B1	20031231	PL 1996-325312	19960827
	ZA 9607379	A	19980330	ZA 1996-7379	19960830
	NO 9800817	A	19980424	NO 1998-817	19980226
	HK 1021532	A1	20020208	HK 1998-114666	19981228
	GR 3036751	T3	20011231	GR 2001-401608	20010928
PRAI	US 1995-3277P	P	19950830		
	WO 1996-US13500	W	19960827		

OS MARPAT 126:264011
AB The title compds. I [A = (un)substituted ureido, guanidino, etc. (generic structures given); Z1 = H, alkyl, OH, alkoxy, halo, (di)(alkyl)amino, aryl, etc.; V = NR6; R6 = H, alkyl, etc.; or YR6 forms a 4- to 12-membered mono-N-containing ring; Y, Y3, Z, Z3 = H, alkyl, aryl, cycloalkyl; or YZ or Y3Z3 form cycloalkyl; n = 1-3; t = 0-2; p = 0-3; R = XR3; X = O, S, NH, etc.; R3 = H, alkyl, etc.; R1 = H, alkyl, alkenyl, etc.; R11 = H, alkyl, aralkyl, etc.] are prepared For example, m-nitrohippuric acid was subjected to a sequence of (1) amidation with Et 3-amino-3-(3-pyridyl)propanoate-

2HCl; (2) hydrogenation of the nitro group; (3) reaction of the formed amine with benzyl isocyanate; and (4) alkaline saponification of the ester, to give
title compound II, isolated as the CF3CO2H or HCl salt. In an in vitro assay for antagonism of human vitronectin receptor (αVβ3), the title compound II.HCl bound with an IC50 of 0.86 nM.

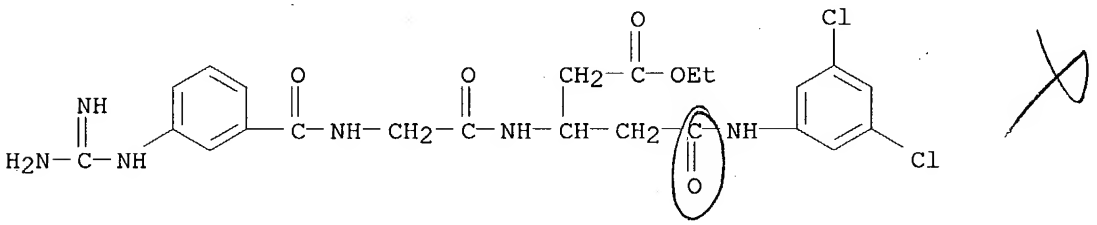
IT **188810-81-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of meta-guanidino, -ureido, -thioureido, or -azacyclic-amino benzoic acid derivs. as integrin antagonists)

RN 188810-81-3 CAPLUS

CN Pentanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-5-[(3,5-dichlorophenyl)amino]-5-oxo-, ethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

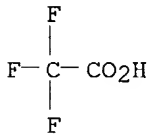
CM 1

CRN 188810-80-2
CMF C23 H26 Cl2 N6 O5



CM 2

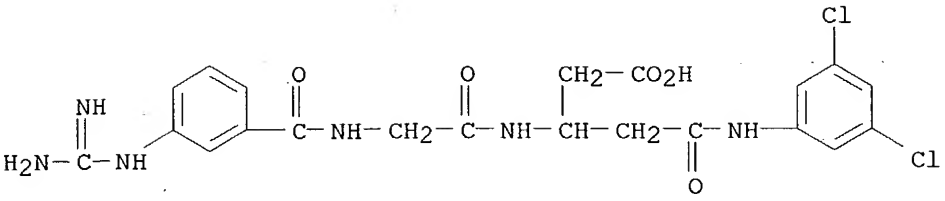
CRN 76-05-1
CMF C2 H F3 O2



IT **188809-64-5P 188809-65-6P 188810-80-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of meta-guanidino, -ureido, -thioureido, or -azacyclic-amino benzoic acid derivs. as integrin antagonists)

RN 188809-64-5 CAPLUS

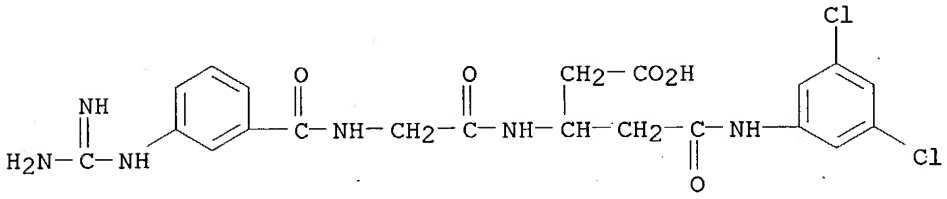
CN Pentanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-5-[(3,5-dichlorophenyl)amino]-5-oxo- (9CI) (CA INDEX NAME)



RN 188809-65-6 CAPLUS
CN Pentanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-5-[(3,5-dichlorophenyl)amino]-5-oxo-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

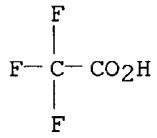
CM 1

CRN 188809-64-5
CMF C21 H22 Cl2 N6 O5

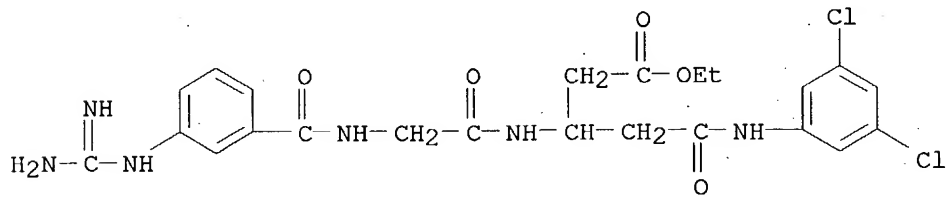


CM 2

CRN 76-05-1
CMF C2 H F3 O2

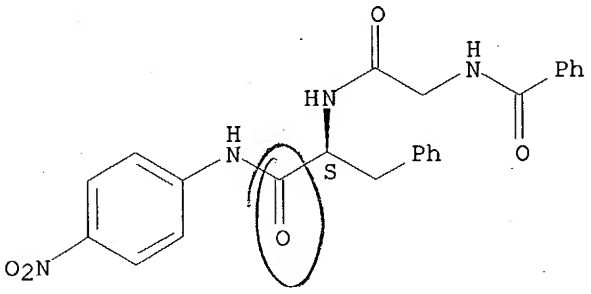


RN 188810-80-2 CAPLUS
CN Pentanoic acid, 3-[[[[3-[(aminoiminomethyl)amino]benzoyl]amino]acetyl]amino]-5-[(3,5-dichlorophenyl)amino]-5-oxo-, ethyl ester (9CI) (CA INDEX NAME)



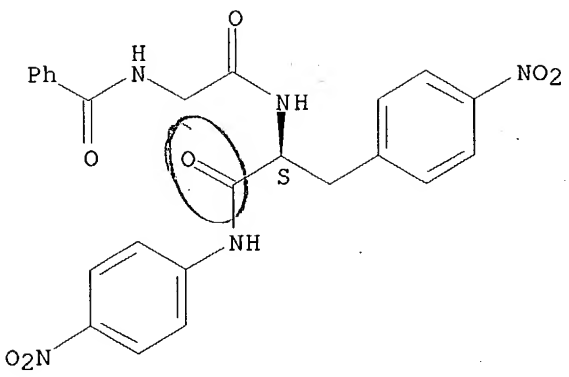
L71 ANSWER 9 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:248791 CAPLUS
DN 126:327291
TI Design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites
AU Portaro, Fernanda C. V.; Cezari, Maria H. S.; Juliano, Maria A.; Juliano, Luiz; Walmsley, Adrian R.; Prado, Eline S.
CS Department Biophysics, Universidade Federal Sao Paulo-Escola Paulista Medicina, Sao Paulo, 04044-020, Brazil
SO Biochemical Journal (1997), 323(1), 161-171
CODEN: BIJOAK; ISSN: 0264-6021
PB Portland Press
DT Journal
LA English
AB Tissue kallikrein inhibitors were derived by selectively replacing residues in Nα-substituted arginine- or phenylalanine-pNA (where pNA is p-nitroanilide), and in peptide substrates for these enzymes. Phenylacetyl-Arg-pNA was an efficient inhibitor of human tissue kallikrein (Ki 0.4 μM) and was neither a substrate nor an inhibitor of plasma kallikrein. The peptide inhibitors having phenylalanine as the P1 residue behaved as specific inhibitors for kallidin-releasing tissue kallikreins, whereas plasma kallikrein showed high affinity for inhibitors containing (p-nitro)phenylalanine at the same position. The Ki value of the most potent inhibitor developed, Abz-Phe-Arg-Arg-Pro-Arg-EDDnp [where Abz is o-aminobenzoyl and EDDnp is N-(2,4-dinitrophenyl)-ethylenediamine], was 0.08 μM for human tissue kallikrein. Progress curve analyses of the inhibition of human tissue kallikrein by benzoyl-Arg-pNA and phenylacetyl-Phe-Ser-Arg-EDDnp indicated a single-step mechanism for reversible formation of the enzyme-inhibitor complex.
IT **189621-44-1 189621-45-2**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(design of kallidin-releasing tissue kallikrein inhibitors based on the specificities of the enzyme's binding subsites)
RN 189621-44-1 CAPLUS
CN L-Phenylalaninamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 189621-45-2 CAPLUS
CN L-Phenylalaninamide, N-benzoylglycyl-4-nitro-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

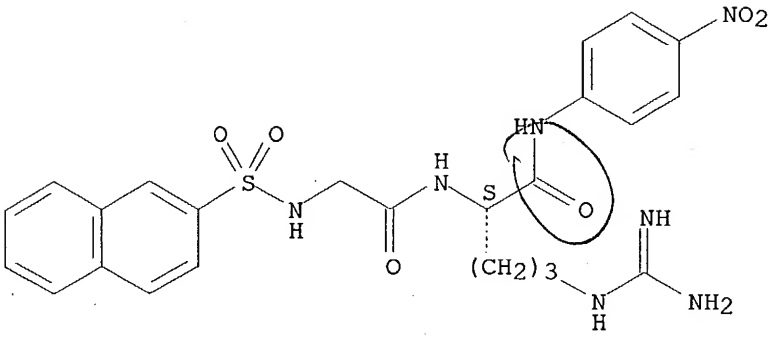
L71 ANSWER 10 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:560491 CAPLUS
DN 125:215690
TI Methods of determining endogenous thrombin potential and thrombin substrates for use in said methods
IN Hemker, Hendrik Coenraad; Rijkers, Dirk Thomas Sigurd; Tesser, Godefriedus Ignatius
PA Neth.
SO PCT Int. Appl., 113 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9621740	A1	19960718	WO 1996-NL18	19960110
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN				
	AU 9646348	A1	19960731	AU 1996-46348	19960110
	EP 802986	A1	19971029	EP 1996-902007	19960110
	EP 802986	B1	20010919		
	R: CH, DE, ES, FR, GB, IT, LI, NL				
	ES 2162025	T3	20011216	ES 1996-902007	19960110
	US 6207399	B1	20010327	US 1997-860808	19970905
PRAI	EP 1995-200043	A	19950110		
	WO 1996-NL18	W	19960110		

OS MARPAT 125:215690
AB A method for determining the ETP (endogenous thrombin potential) of a sample, preferably in a continuous assay is claimed, said sample comprising a total anticoagulant activity of or equivalent to at least 0,07 U ISH/mL, wherein a thrombin substrate or a salt thereof that is soluble in the sample is applied in a manner known per se for determining the ETP of a sample, said thrombin substrate being selected from the group comprising substrates of the formula P-Val-Xaa-S (P = nonarom., polar amino protective group; Val = valine residue attached via a peptide bond to Xaa; Xaa = amino acid residue comprising a terminal guanidino group or ureido group separated by at least 2 carbon atoms from the peptide backbone, said amino acid residue being attached to S; S = signal group such as a chromophore that can be enzymically hydrolyzed). Other substrates such as Zaa-Pipecolyl-Yaa-S or Zaa-Pro-Yaa-S, (Zaa = D-Phe, D-Trp, D-Tyr; Pro = proline; Yaa = amino acid residue other than Arg; S = signal group) can also be used. The substrates Boc-Gly-Val-Arg-pNA and H-Glu-Gly-Val-Arg-pNA are also applicable. Furthermore ETP determination methods as such can be improved by addition of hydroxylamine to the sample to circumvent defibrination of the sample.
IT **167961-66-2P**
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(methods of determining endogenous thrombin potential and thrombin substrates
for use in said methods)
RN 167961-66-2 CAPLUS
CN L-Argininamide, N-(2-naphthalenylsulfonyl)glycyl-N-(4-nitrophenyl)-,

monohydrochloride (9CI) (CA INDEX NAME)

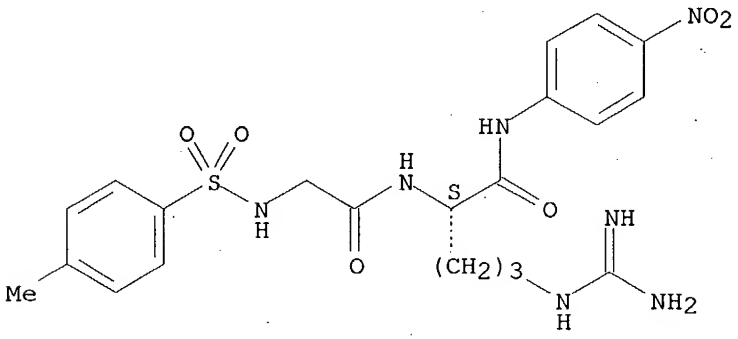
Absolute stereochemistry.



● HCl

IT **167961-67-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(methods of determining endogenous thrombin potential and thrombin substrates
for use in said methods)
RN 167961-67-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



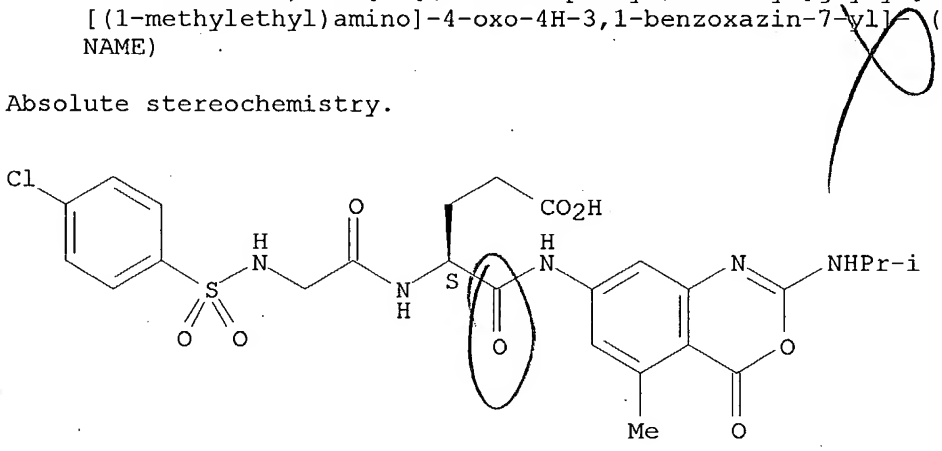
● HCl

L71 ANSWER 11 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:241536 CAPLUS
DN 124:290265
TI Preparation of amino acid moiety-containing benzoxazines as elastase inhibitors
IN Oshida, Junichi; Kawabata, Hiroshi; Kato, Yoshinori; Kokubo, Masayuki; Ueshima, Yasuhide; Sato, Osami; Fujii, Katsuhiko
PA Teijin Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 34 pp. Division of Jpn. Kokai Tokkyo Koho Appl. NO. 91 504,791.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 07316056	A2	19951205	JP 1994-272320	19941107
PRAI JP 1991-504791		19910215		

OS MARPAT 124:290265
AB The title compds. I [R1 = H, alkyl; X = Y1A1, Y2(A2)mA3; when X is Y1A1 : R2, R3 = H, (carboxy)alkyl, or NR2R3 = ring; when X is Y2(A2)mA3 : R2 = alkyl, R3 = H; Y1 = amino-protecting group; Y2 = H, sulfonyl; A1, A2 = amino acid residue, etc.; A3 = lysine residue, etc.; m = 0 or 1] are prepared 7-(N-benzyloxycarbonyl-L-phenylalanyl)amino-5-methyl-2-(1-carboxyethyl)amino-4H-3,1-benzoxazin-4-one (preparation given) in vitro showed IC50 values of 5.1 x 10-8 M and 1.5 x 10-6 M against elastase and chymotrypsin, resp.
IT **138006-83-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid moiety-containing benzoxazines as elastase inhibitors)
RN 138006-83-4 CAPLUS
CN L-α-Glutamine, N2-[N-[(4-chlorophenyl)sulfonyl]glycyl]-N-[5-methyl-2-[(1-methylethyl)amino]-4-oxo-4H-3,1-benzoxazin-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

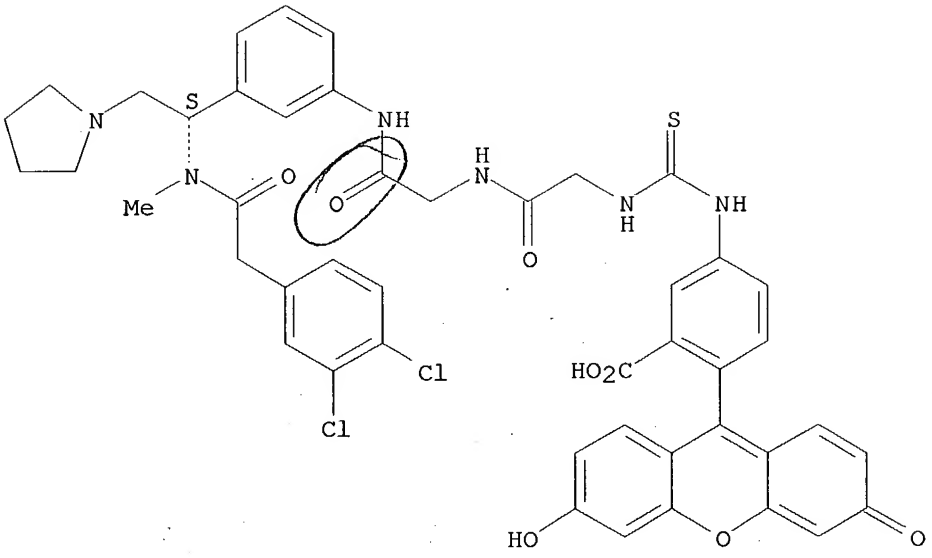


L71 ANSWER 12 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:175894 CAPLUS
DN 124:254974
TI Arylacetamide-derived fluorescent probes: synthesis, biological evaluation, and direct fluorescent labeling of κ opioid receptors in mouse microglial cells
AU Chang, An-Chih; Chao, Chun C.; Takemori, Akira E.; Gekker, Genya; Hu, Shuxian; Peterson, Phillip K.; Portoghese, Philip S.
CS College of Pharmacy, University of Minnesota, Minneapolis, MN, 55455, USA
SO Journal of Medicinal Chemistry (1996), 39(8), 1729-35
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB Fluorescein isothiocyanate isomer I (FITC-I) conjugates of 2-(3,4-dichlorophenyl)-N-methyl-N-[1-(3- or 4-aminophenyl)-2-(1-pyrrolidinyl)ethyl]acetamide (10 and 14) were prepared either without or with an intervening mono-, di-, or tetraglycyl linker. The 3-substituted fluorescent probes (2-5) were found to retain potent agonist activity in smooth muscle prepns. as well as high κ receptor affinity and selectivity in receptor binding assays. The 4-substituted series (6-9) were substantially less potent than the corresponding 3-substituted compds. Flow cytometric anal. demonstrated high levels of direct κ-specific staining of mouse microglial cells by the fluorescent probe 5 containing a tetraglycyl linker, as indicated by a 41% decrease in percent cells pos. labeled and a 61% decrease in mean fluorescence intensity in the presence of the κ-selective antagonist, norbinaltorphimine (norBNI). In similar studies, the probe 2 without a linker exhibited only nonspecific binding. This is the first report of direct, selective staining of κ opioid receptors by a fluorescent nonpeptide opioid ligand. The results of the present study illustrate the importance of introducing hydrophilic linkers to reduce nonspecific binding of fluorescent probes for opioid receptors.
IT **174971-79-0P 174971-87-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(arylacetamide-derived fluorescent probes synthesis, smooth muscle agonist activity, and direct fluorescent labeling of κ opioid receptors in mouse microglial cells)
RN 174971-79-0 CAPLUS
CN Glycinamide, N-[[[3-carboxy-4-(6-hydroxy-3-oxo-3H-xanthen-9-yl)phenyl]amino]thioxomethyl]glycyl-N-[3-[1-[[(3,4-dichlorophenyl)acetyl]methylamino]-2-(1-pyrrolidinyl)ethyl]phenyl]-, (S)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

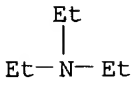
CRN 174971-78-9
CMF C46 H42 Cl2 N6 O8 S

Absolute stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N

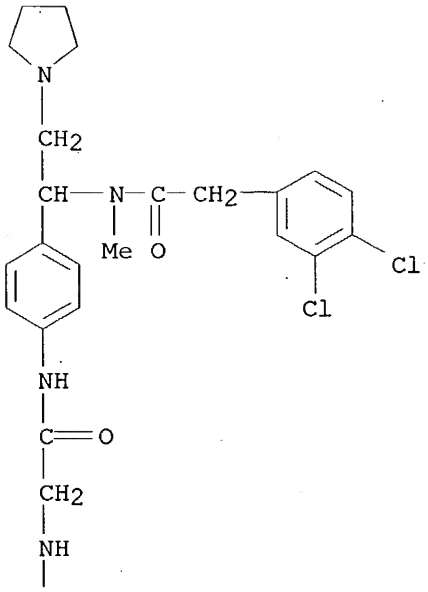


RN 174971-87-0 CAPLUS
CN Glycinamide, N-[[[3-carboxy-4-(6-hydroxy-3-oxo-3H-xanthen-9-yl)phenyl]amino]thioxomethyl]glycyl-N-[4-[1-[[(3,4-dichlorophenyl)acetyl]methylamino]-2-(1-pyrrolidinyl)ethyl]phenyl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

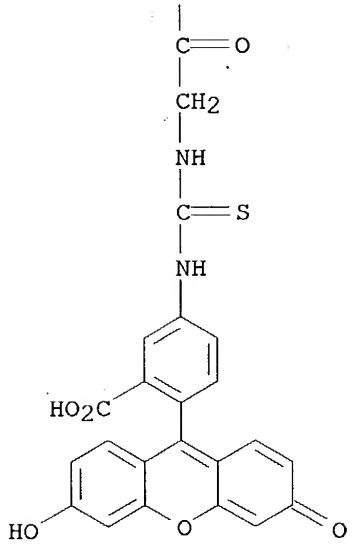
CM 1

CRN 174971-86-9
CMF C46 H42 Cl2 N6 O8 S

PAGE 1-A

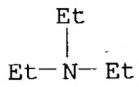


PAGE 2-A



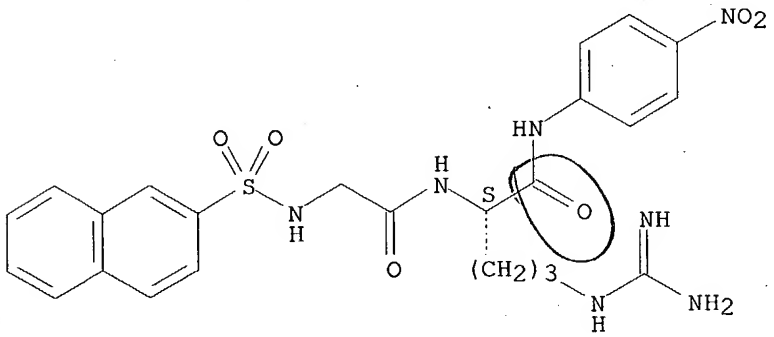
CM 2

CRN 121-44-8
CMF C6 H15 N



L71 ANSWER 13 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:762217 CAPLUS
DN 123:192056
TI Design and synthesis of thrombin substrates with modified kinetic parameters
AU Rijkers, Dirk T. S.; Welders, Simone J. H.; Tesser, Godefridus I.; Hemker, H. Coenraad
CS Faculty of Medicine, University of Limburg, Maastricht, 6200 MD, Neth.
SO Thrombosis Research (1995), 79(5/6), 491-9
CODEN: THBRAA; ISSN: 0049-3848
PB Elsevier
DT Journal
LA English
AB For the continuous registration of thrombin formation in plasma, selective thrombin substrates are required, that show moderate binding affinities (high Km) and low turnover nos. (low kcat). Previously the authors have used SQ68 (CH3O-CO-CH2-CO-Aib-Arg-pNA) for this purpose. To find more substrates suitable for this application, the authors synthesized a series of 25 peptide p-nitroanilides. As lead structures SQ68 and S2238 (H-D-Phe-Pip-Arg-pNA) were used. By introduction of specific structure modifications the authors tried to alter the kinetic data in the required direction. The modifications were designed on basis of existing knowledge on the structure of the thrombin active-site and its surroundings. The authors indeed obtained a number of substrates with the kinetic consts. in the desired range.
IT **167961-66-2P 167961-67-3P**
RL: BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(design and synthesis of peptide p-nitroanilides and reaction with human α-thrombin and factor Xa)
RN 167961-66-2 CAPLUS
CN L-Argininamide, N-(2-naphthalenylsulfonyl)glycyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

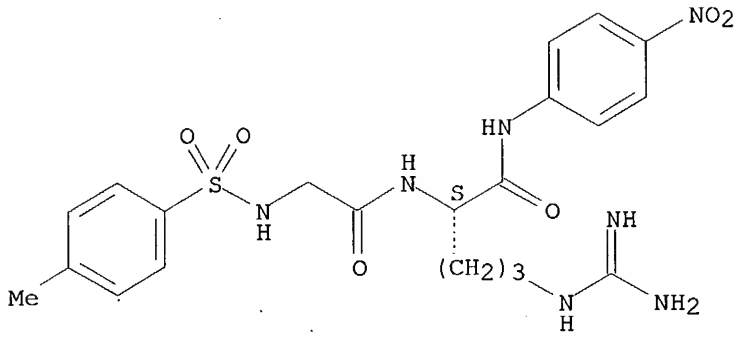
Absolute stereochemistry.



● HCl

RN 167961-67-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

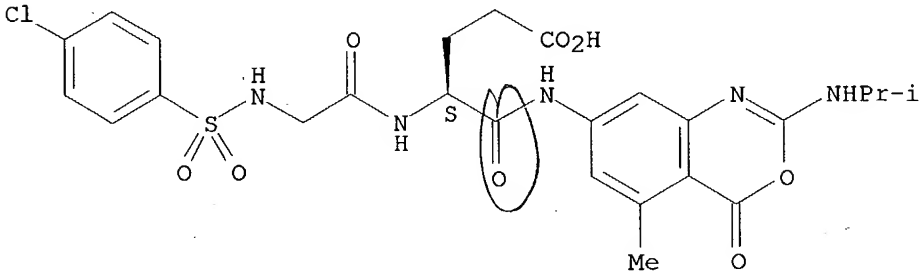
Absolute stereochemistry.



● HCl

L71 ANSWER 14 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1994:646178 CAPLUS
DN 121:246178
TI Inhibition of human sputum elastase by 7-substituted 5-methyl-2-isopropylamino-4H-3,1-benzoxazin-4-ones
AU Uejima, Yasuhide; Oshida, Jun-Ichi; Kawabata, Hiroshi; Kokubo, Masayuki; Kato, Yoshinori; Fujii, Katsuhiko
CS Teijin Institute for Biomedical Research, Tokyo, 191, Japan
SO Biochemical Pharmacology (1994), 48(2), 426-8
CODEN: BCPCA6; ISSN: 0006-2952
DT Journal
LA English
AB 7-Substituted 5-methyl-2-isopropylamino-4H-3,1-benzoxazin-4-ones (BOZNs) were prepared and tested as inhibitors of human sputum elastase (HSE). The BOZNs with certain amino acid residues at the 7-position proved to be potent inhibitors of HSE. Some of the compds. also showed a high selectivity for HSE vs. chymotrypsin. In a hamster model in which acute injury was induced by intratracheal administration of HSE (1.0 mg/kg), these compds., when administered intratracheally (1.0 mg/kg) either 30 or even 240 min before challenge with HSE, significantly suppressed pulmonary hemorrhage. These findings suggest that 7-substitution of BOZN by amino acid residues can produce strong and HSE-specific inhibitors, with potential use in elastase-mediated disorders.
IT **138006-83-4**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of human sputum elastase by 7-substituted 5-methyl-2-isopropylamino-4H-3,1-benzoxazin-4-ones)
RN 138006-83-4 CAPLUS
CN L-α-Glutamine, N2-[N-[(4-chlorophenyl)sulfonyl]glycyl]-N-[5-methyl-2-[(1-methylethyl)amino]-4-oxo-4H-3,1-benzoxazin-7-yl]- (9CI) (CA INDEX NAME)

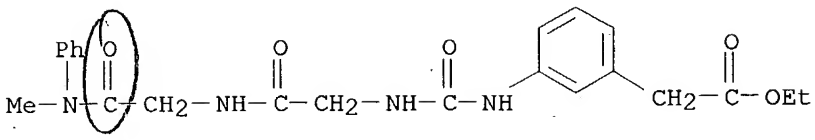
Absolute stereochemistry.



L71 ANSWER 15 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:106815 CAPLUS
DN 116:106815
TI Preparation of derivatives of N-phenylglycinamide as CCK and gastrin antagonists.
IN Bourzat, Jean Dominique; Capet, Marc; Cotrel, Claude; Guyon, Claude; Manfre, Franco; Roussel, Gerard
PA Rhone-Poulenc Rorer SA, Fr.
SO PCT Int. Appl., 100 pp.
CODEN: PIXXD2
DT Patent
LA French
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9113907	A1	19910919	WO 1991-FR174	19910305
	W: AU, CA, HU, JP, KR, NO, SU, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
	FR 2659334	A1	19910913	FR 1990-2889	19900307
	FR 2659334	B1	19920515		
	FR 2667864	A2	19920417	FR 1990-12727	19901016
	FR 2667864	B2	19940805		
	AU 9174920	A1	19911010	AU 1991-74920	19910305
	AU 635832	B2	19930401		
	EP 518960	A1	19921223	EP 1991-905832	19910305
	EP 518960	B1	19940914		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	HU 61576	A2	19930128	HU 1992-2865	19910305
	JP 05504967	T2	19930729	JP 1991-505781	19910305
	ES 2059128	T3	19941101	ES 1991-905832	19910305
	RU 2076108	C1	19970327	RU 1991-5053153	19910305
	ZA 9101637	A	19911224	ZA 1991-1637	19910306
	IL 97476	A1	19960723	IL 1991-97476	19910307
	NO 9203456	A	19920904	NO 1992-3456	19920904
	US 5475106	A	19951212	US 1992-924065	19921008
PRAI	FR 1990-2889		19900307		
	FR 1990-12727		19901016		
	WO 1991-FR174		19910305		

OS MARPAT 116:106815
AB R2COCHR1NR4COCH2NHCOR3 [I; R1 = H, alkyl, alkoxycarboyl, (substituted) phenyl; R2 = alkoxy, (substituted) cycloalkoxy, cycloalkylalkoxy, phenylalkoxy, polyfluoroalkoxy, cinnamyloxy, (substituted) amino; R3 = (substituted) phenylamino, etc.; R4 = Ph substituted by a halogen, alkyl, alkoxy, etc.], useful as antagonists against CCK and gastrin (no data), are prepared N-(Chlorophenyl)acetamide II [R5 = H] (preparation given) in THF was reacted with m-MeC6H4NCO at 20° to give II [R5 = m-MeC6H4NHCO]. Tablets, injections, etc., containing I were formulated.
IT **139089-29-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for CCK and gastrin antagonists)
RN 139089-29-5 CAPLUS
CN Benzeneacetic acid, 3-[[[[2-[[2-(methylphenylamino)-2-oxoethyl]amino]-2-oxoethyl]amino]carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

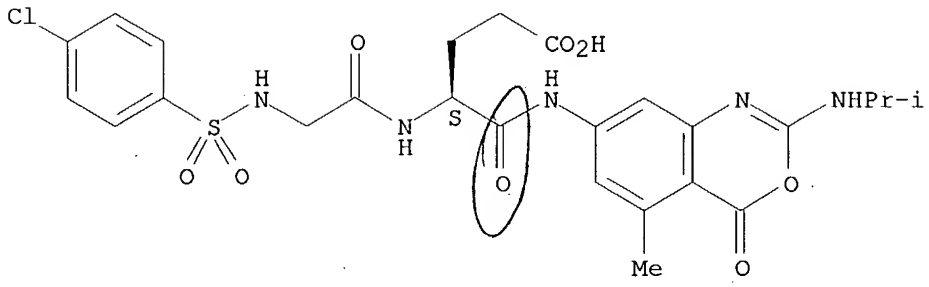


L71 ANSWER 16 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1992:21062 CAPLUS
DN 116:21062
TI Preparation of 7-(peptidylamino)-4H-3,1-benzoxazin-4-one compound and elastase inhibitor composition containing same
IN Oshida, Junichi; Kawabata, Hiroshi; Kato, Yoshinori; Kokubo, Masayuki; Uejima, Yasuhide; Sato, Osami; Fujii, Katsuhiko
PA Teijin Ltd., Japan
SO PCT Int. Appl., 101 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9112245	A1	19910822	WO 1991-JP183	19910215
	W: AU, CA, JP, KR, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, NL, SE				
	CA 2051115	AA	19910816	CA 1991-2051115	19910215
	AU 9173250	A1	19910903	AU 1991-73250	19910215
	AU 635403	B2	19930318		
	EP 466944	A1	19920122	EP 1991-904621	19910215
	R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
PRAI	JP 1990-32440		19900215		
	WO 1991-JP183		19910215		

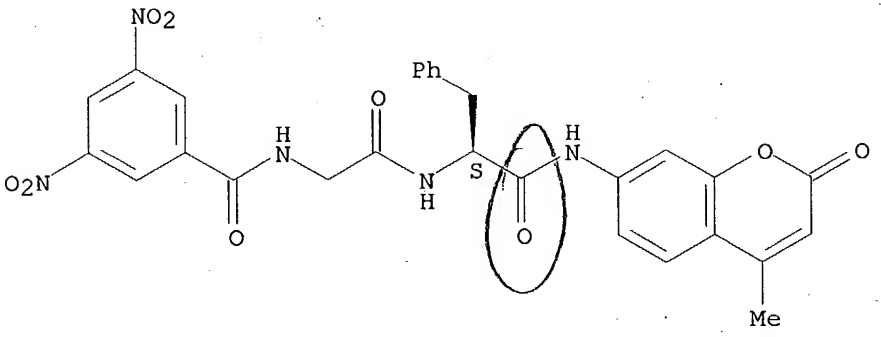
OS MARPAT 116:21062
AB The title compds. [I; X = Y1A1, Y2(A2)mA3; A1 = amino acid residue, peptide residue comprising 2 or 3 amino acid residues; A2 = Gly, Ala, Val, Leu, dipeptide residue containing these amino acid residues; A3 = (side-chain protected) Lys, Glu, Or Asp; Y1 = amino-protecting group; Y2 = H, SO3H; provided that when the side-chain of A3 is protected , Y2 = H; m = 0, 1; when X = Y1A1, R2 = alkyl containing 1 or 2 CO2H, and R3 = H, alkyl containing 1
or 2 alkyl or CO2H, or NR2R3 forming a 6- to 7-membered ring optionally substituted with 1 or 2 alkyl or CO2H; when X = Y2(A2)mA3, R2 = alkyl and R3 = H], which show particularly a selective inhibiting effect on a human leukocyte elastase and excellent H2O-solubility and residence in the lung tissue, are prepared Thus, treatment of BOC-LysCOCMe3)-OH with iso-BuO2CCl in THF containing N-methylmorpholine at -15° followed by I (R1 = Me, R2 = Me2CH, R3 = X = H) (preparation given) gave I [R1,R2,R3 = unchanged; X = BOC-Lys(OCM33)] which was deprotected with 4N HCl in dioxane, treated with Me3SiNHNHSiMe3 in CH2Cl2, and then condensed with 4-ClC6H4SO2Cl in the presence of Et3N to give I [R1,R2,R3 = unchanged; X = p-ClC6H4SO2-Lys] (II). II in vitro inhibited human purulent sputum elastase and α-chymotrypsin with IC50 of 2.9 + 10-9 and 4.9 + 10-6 M and 1690 times selectivity for the elastase.
IT **138006-83-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as elastase inhibitor)
RN 138006-83-4 CAPLUS
CN L-α-Glutamine, N2-[N-[(4-chlorophenyl)sulfonyl]glycyl]-N-[5-methyl-2-[(1-methylethyl)amino]-4-oxo-4H-3,1-benzoxazin-7-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


Cl
O
H
N
S
O
O
N
H
S
CO2H
O
H
N
N
NHPr-i
O
Me
O

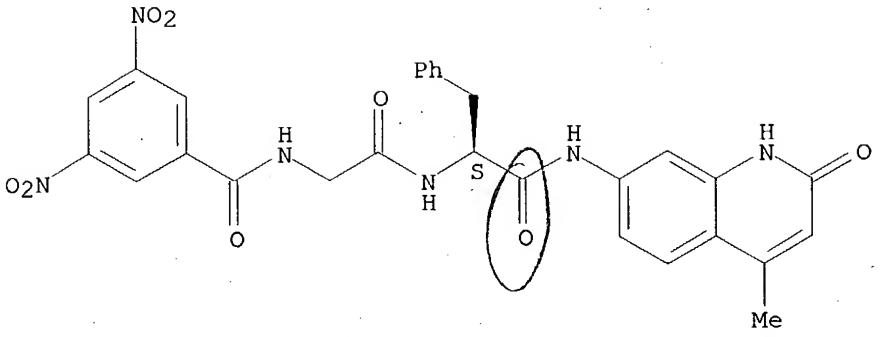
L71 ANSWER 17 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:409314 CAPLUS
DN 115:9314
TI Synthesis and study of intramolecularly-quenched fluorogenic substrates containing aminocoumarin or aminoquinolinone-type fluorophores
AU Kokotos, George; Tzougraki, Chryssa
CS Dep. Chem., Univ. Athens, Athens, 15771, Greece
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1991), (4), 495-9
CODEN: JCPKBH; ISSN: 0300-9580
DT Journal
LA English
AB Quenched fluorogenic substrates I and II [X = NH, O; R = 2,4-(O2N)2C6H3 (Dnp), 2,4,6-(O3N)3C6H2 (Tnp), 2-O2NC6H4S (Nps), 3,5-(O2N)2C6H3CO] were prepared Efficient quenching of fluorescence is observed in all cases. The Dnp, Nps, and Tnp groups show a higher quenching efficiency and II (R = Dnp) gives the best result (99% quenching). The substrates synthesized can be used for the direct specific determination of enzymes which hydrolyze the peptide chain at any point between the interacting groups by measuring the increase in fluorescence.
IT **134269-02-6P 134269-06-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and fluorescence of)
RN 134269-02-6 CAPLUS
CN L-Phenylalaninamide, N-(3,5-dinitrobenzoyl)glycyl-N-(4-methyl-2-oxo-2H-1-benzopyran-7-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 134269-06-0 CAPLUS
CN L-Phenylalaninamide, N-(3,5-dinitrobenzoyl)glycyl-N-(1,2-dihydro-4-methyl-5-oxo-7-quinolinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

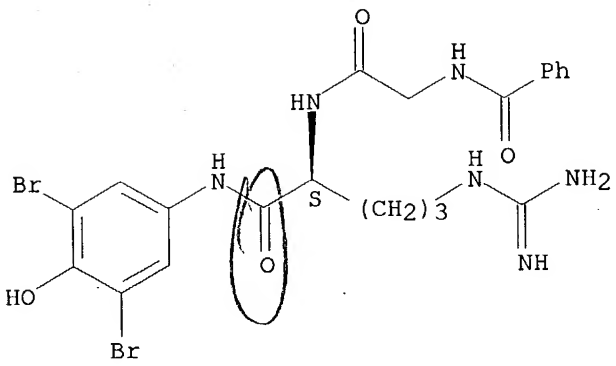

NO2
O2N
O
H
N
O
N
H
Ph
S
O
H
N
H
N
O
Me

L71 ANSWER 18 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:154777 CAPLUS
DN 112:154777
TI Composition or kit containing peptide substrates for testing periodontal diseases by determining peptidase-like enzymic activity
IN Suido, Hirohisa; Miike, Akira; Hasegawa, Kenji; Kayahara, Norihiko; Eguchi, Toru; Tatano, Toshio; Nakashima, Koichi
PA Sunstar, Inc., Japan; Kyowa Medex Co., Ltd.
SO Eur. Pat. Appl., 18 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 325472	A2	19890726	EP 1989-300533	19890120
	EP 325472	A3	19900620		
	EP 325472	B1	19930428		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 02000499	A2	19900105	JP 1988-331988	19881228
	JP 06050995	B4	19940706		
	AT 88759	E	19930515	AT 1989-300533	19890120
	ES 2055029	T3	19940816	ES 1989-300533	19890120
	CA 1332347	A1	19941011	CA 1989-588832	19890120
	KR 140216	B1	19980601	KR 1989-615	19890120
	US 5223404	A	19930629	US 1991-639742	19910111
PRAI	JP 1988-10241	A	19880120		
	JP 1988-331988	A	19881228		
	US 1989-298965	B1	19890119		
	EP 1989-300533	A	19890120		

OS MARPAT 112:154777
AB The title composition or kit comprises (1) peptide derivs. X-T-Pro-Y and/or X-Z-Arg-Y (X = H, amino protecting group; Y is a residue of a compound capable of increasing the oxidation rate of a chromogen with an oxidase in the presence of O; T, Z = amino acid, peptide containing 0-4 amino acids or their protected derivs.); (2) a chromogen; and (3) an oxidase. The enhancer residue Y may be an aniline derivative Saliva samples from healthy subjects and patients with periodontitis and juvenile periodontitis were centrifuged and the supernatants were tested for hydrolytic activity using N-carbobenzoxy-glycyl-arginine-DIHA (DIHA = 3,5-diiodo-4-hydroxyanilinyl) and N-benzoyl-arginyl-glycyl-phenylalanyl-proline-DIHA, alone or in combination, as substrates, ascorbate oxidase, and I. The diseased group showed .gtorsim.1.5 times higher activity than the healthy group when both substrates were used. The values were 10 times higher than those of a conventional method.
IT **126152-05-4**
RL: ANST (Analytical study)
(as substrate, in peptidase assay for periodotal disease diagnosis)
RN 126152-05-4 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(3,5-dibromo-4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

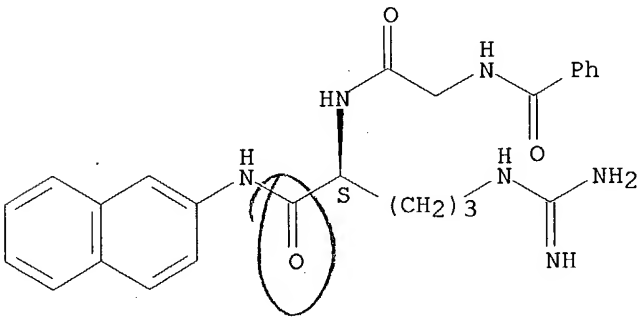

O
H
N
Ph
HN
O
H
N
NH2
Br
S
(CH2)3
NH
O
HO
Br

L71 ANSWER 19 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:84179 CAPLUS
DN 112:84179
TI Aminopeptidase and its substrates for the diagnosis of gingivitis
IN Eguchi, Toru; Suido, Hirohisa; Nakajima, Koichi; Hasegawa, Kenji; Kanbara, Mitsuho; Nakamura, Shoichi
PA Sunstar, Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 01014000	A2	19890118	JP 1987-170779	19870708
	JP 06050993	B4	19940706		
PRAI	JP 1987-170779		19870708		

OS MARPAT 112:84179
AB A diagnostic agent for gingivitis contains X-T-Pro-S (Pro = proline residue; X = H or amino group protector; S = a luminating group which binds to the C-terminal of the proline residue; T = 0-4 amino acid or derivative which binds to the N-terminal of the proline residue) and X-Z-Arg-Y (Arg = arginine residue; X = H or NH2 protecting group; Y = a luminating agent binding to C terminal of Pro; Z = 0-4 amino acid or its protective derivative). These agents are substrates of aminopeptidase, and the measurement of the enzyme activity shows the extent of gingivitis in patients oral cavities. Thus, N-carbobenzoxy-glycyl-glycyl-arginine-β-naphthylamide (20 mM) solution was prepared in a 0.1 M tris-HCl buffer (pH 7.0) and added to a nitrocellulose filter. This filter was used in the detection of aminopeptidase activity associated with dental plaque bacteria.
IT **115871-03-9**
RL: BIOL (Biological study)
(as aminopeptidase substrate, in gingivitis diagnosis)
RN 115871-03-9 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-2-naphthalenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

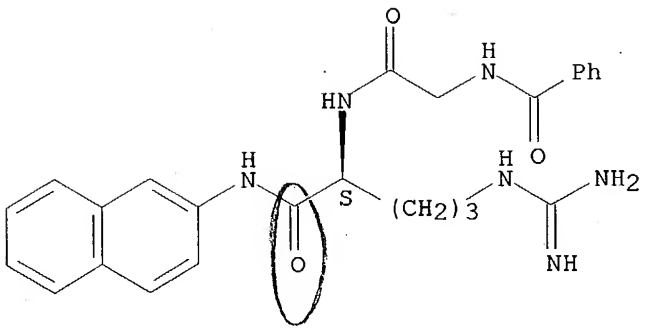


L71 ANSWER 20 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:489350 CAPLUS
DN 109:89350
TI Peptide-linked β-naphthylamide derivative reagent for detection of oral pathogens
IN Tanaka, Toshiyuki; Nakamura, Masakazu; Suido, Hirohisa
PA Sunstar, Inc., Japan
SO Eur. Pat. Appl., 24 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

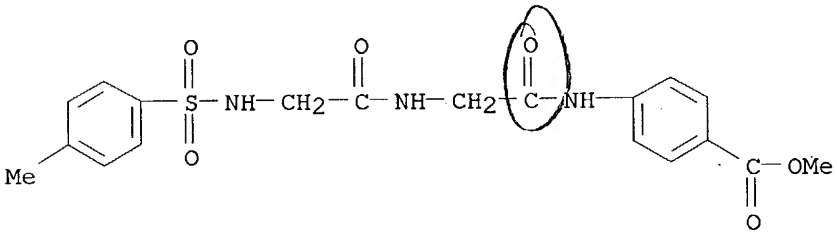
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 255341	A2	19880203	EP 1987-306663	19870728
	EP 255341	A3	19900131		
	EP 255341	B1	19930203		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	JP 63036800	A2	19880217	JP 1986-179716	19860729
	JP 06048998	B4	19940629		
	JP 63087999	A2	19880419	JP 1986-233848	19860930
	JP 06011240	B4	19940216		
	JP 63277966	A2	19881115	JP 1987-113122	19870509
	JP 2516365	B2	19960724		
	AT 85362	E	19930215	AT 1987-306663	19870728
	ES 2053547	T3	19940801	ES 1987-306663	19870728
	CA 1310893	A1	19921201	CA 1987-543277	19870729
	US 5137811	A	19920811	US 1989-459185	19891229
PRAI	JP 1986-179716		19860729		
	JP 1986-233848		19860930		
	JP 1987-113122		19870509		
	JP 1987-233848		19860930		
	US 1987-76875		19870723		
	EP 1987-306663		19870728		

OS MARPAT 109:89350
AB Peptides of formula X-Z-Arg-Y and X-Z'-Pro-Y (X = H, amino blocking group; Y = color developing group; Z = peptide of 1-4 residues; Z' = peptide of 0-4 residues) are substrates for aminopeptidases produced by pathogenic oral microorganisms such as spirochetes and gram-neg. anaerobic bacteria, and are useful for detection of periodontal disease. Specimens of gingival crevicular fluid were collected with paper points from subjects with gingivitis and periodontitis and dispersed in Ringer's solution The specimens were tested for hydrolytic activity with N-benzoylvalylglycylarginine β-naphthylamide and N-carbobenzoxyvalylglycylarginine β-naphthylamide by observation of color development after addition of garnet GBC diazonium salt. Specimens from all patients with periodontitis were strongly pos., those from patients with gingivitis were neg. or weakly pos., and those from normal subjects were almost always neg.
IT **115871-03-9**
RL: ANST (Analytical study)
(as aminopeptidase substrate, for periodontal disease diagnosis)
RN 115871-03-9 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-2-naphthalenyl- (9CI) (CA INDEX NAME)

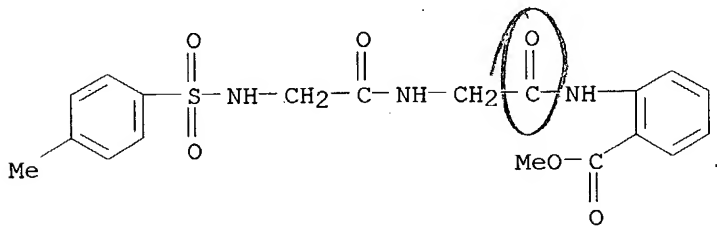
Absolute stereochemistry.


O
H
N
Ph
HN
H
N
O
NH2
S
(CH2)3
O
NH

L71 ANSWER 21 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1988:38341 CAPLUS
DN 108:38341
TI Synthesis of some peptides containing methyl o- and p-aminobenzoate, aminobenzamide, phthalamide and terephthalamide residues
AU El-Naggar, A. M.; Zaher, M. R.; Kora, F. A.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Egyptian Journal of Chemistry (1986), Volume Date 1985, 28(1), 47-52
CODEN: EGJCA3; ISSN: 0367-0422
DT Journal
LA English
AB Tos-Gly-Gly-X-o-Aba-OMe (Tos = tosyl; Aba = aminobenzoic acid residue; X = null, Gly) and Tos-Gly-Gly-X-p-Aba-Ome (X = null, Gly) were prepared by coupling Tos-Gly-Gly-X-OH with H-o-Aba-OMe or H-p-Aba-OMe by DCC. N,N'-Dipeptidyl derivs. of o- and p-aminobenzamide, phthalamide, and terephthalamide were also prepared The above peptides formed complexes with Cu(II). The above peptides and their Cu(II) complexes were inactive against several bacteria, e.g., Bacillus subtilis.
IT **112129-75-6P 112129-76-7P 112129-79-0P 112129-80-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 112129-75-6 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[4-(methoxycarbonyl)phenyl]- (9CI) (CA INDEX NAME)

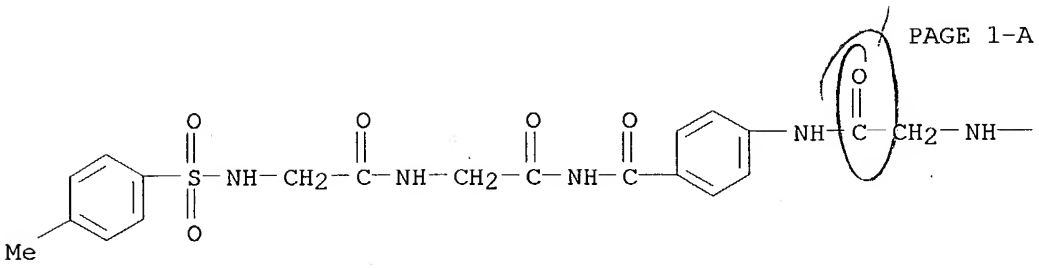


RN 112129-76-7 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[2-(methoxycarbonyl)phenyl]- (9CI) (CA INDEX NAME)

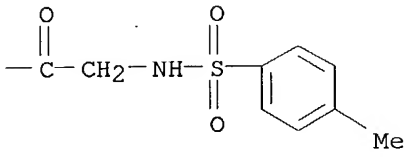


RN 112129-79-0 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[4-[[N-[N-[(4-methylphenyl)sulfonyl]glycyl]glycyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

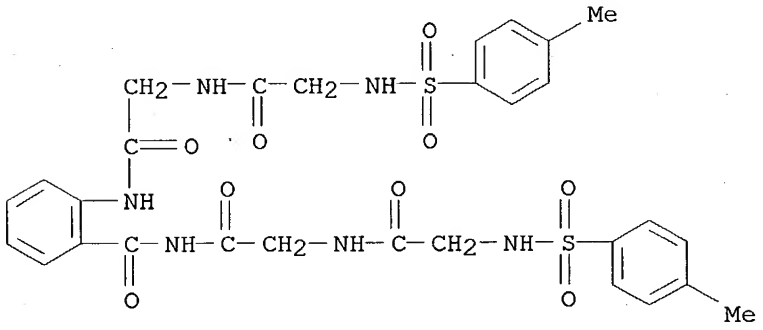
PAGE 1-A



PAGE 1-B

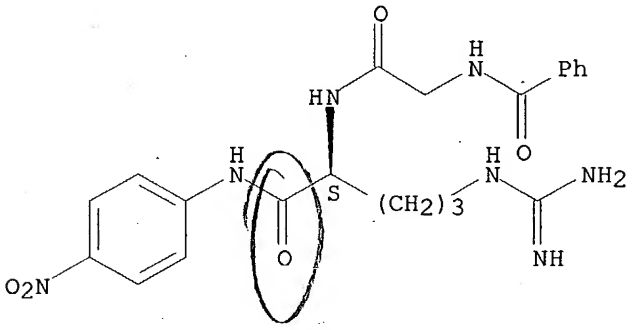


RN 112129-80-3 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-[2-[[N-[N-[(4-methylphenyl)sulfonyl]glycyl]glycyl]amino]benzoyl]- (9CI) (CA INDEX NAME)



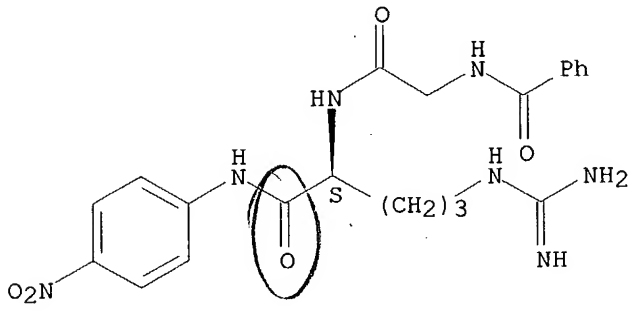
L71 ANSWER 22 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:532277 CAPLUS
DN 107:132277
TI The complement component C.hivin.1s catalyzed hydrolysis of peptide 4-nitroanilide substrates
AU Keogh, Shelley J.; Harding, David R. K.; Hardman, Michael J.
CS Dep. Chem. Biochem., Massey Univ., Palmerston North, N. Z.
SO Biochimica et Biophysica Acta (1987), 913(1), 39-44
CODEN: BBACAQ; ISSN: 0006-3002
DT Journal
LA English
AB The kinetic parameter kcat/Km was determined for the hydrolysis of peptide 4-nitroanilides, catalyzed by complement component C.hivin.1s. Substrates based on the C-terminal sequence of human C4a (Leu-Gln-Arg) were synthesized. Replacement of the glutamine residue by glycine or serine increased kcat/Km. Substitution of valine for the leucine residue increased kcat/Km, while substitution of glycine or lysine for the leucine residue decreased kcat/Km slightly. D-Val-Ser-Arg 4-nitroanilide is the most reactive substrate towards C.hivin.1s, so far. These results are discussed in relation to the amino acid sequences near the bonds cleaved by C.hivin.1s in C4, C2, and C.hivin.1 inhibitor.
IT **103418-67-3P**
RL: PREP (Preparation)
(preparation and hydrolysis by complement C1 components)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

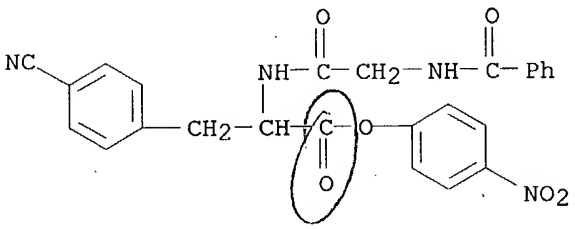


L71 ANSWER 23 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:605278 CAPLUS
DN 105:205278
TI Synthesis and kinetic parameters of hydrolysis by trypsin of some acyl-arginyl-p-nitroanilides and peptides containing arginyl-p-nitroanilide
AU Juliano, M. A.; Juliano, L.
CS Dep. Biofis., Esc. Paul. Med., Sao Paulo, 04034, Brazil
SO Brazilian Journal of Medical and Biological Research (1985), 18(4), 435-45
CODEN: BJMRDK; ISSN: 0100-879X
DT Journal
LA English
AB Four acyl-arginyl-p-nitroanilides, 9 acetyl-(or benzoyl)-aminoacyl-arginyl-p-nitroanilides and 12 acyl-(or free α-amino-)dipeptidyl-arginyl-p-nitroanilides were synthesized, and the kinetic parameters for tryptic hydrolysis of these substrates were determined in 100 mM Tris-HCl buffer, pH 8.0, containing 10 mM CaCl2 at 37°. Among the acyl-arginyl-p-nitroanilides, octanoyl-Arg-pNA (where pNA=p-nitroanilide and Arg = arginine) was hydrolyzed 4-fold more rapidly by trypsin than the commonly used substrate benzoyl-Arg-pNa. The best trypsin substrates contain proline and noreleucine at subsite P2, indicating that unbranched aliphatic side chain folded as the β, γ, and δ methylenes are in proline provides the most favorable conditions for S2P2 interaction. Extending the length of the substrates from di- to tripeptidyl-pNA did not have a large influence on the kinetic parameters. However, phenylalanine (Phe) at the P3 position had a clear favorable effect, in contrast to proline, which is unfavorable only when the group is present at P4. The series Ac-Phe (or D-Phe)-Gly-Arg-pNA and Phe (or D-Phe)-Gly-Arg-pNA were studied. The benzyl side chain of D-Phe has a more favorable interaction at S3 than Phe (Phe = phenylalanine). A P4-CO...HN-S4 H bond is proposed to stabilize P3/S3 interaction when an acetyl group is present on the α-amino group of the Phe residue, and the reverse would be expected to occur for the corresponding D-epimer.
IT **103418-67-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and trypsin reaction kinetics with)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

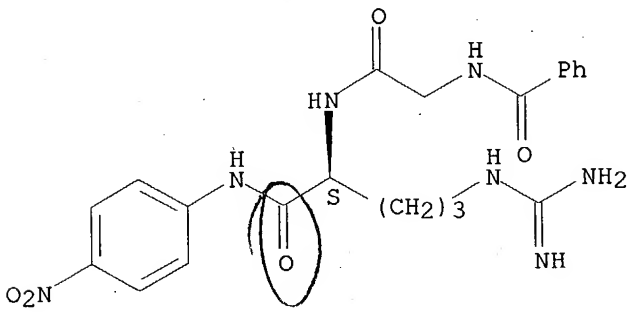


L71 ANSWER 24 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:497888 CAPLUS
DN 105:97888
TI Synthesis of Nα-(benzoylglycyl)- and Nα-(benzyloxycarbonylglycyl)-4-amidinophenylalanine as thrombin inhibitors
AU Voigt, B.; Wagner, G.
CS Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010, Ger. Dem. Rep.
SO Pharmazie (1985), 40(8), 527-9
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
OS CASREACT 105:97888
AB Dipeptides I (R = Bz, PhCH2O2C) were condensed with HNR1R2 (NR1R2 = piperidino, pyrrolidino, morpholino, NBu) to give dipeptide amides II (R, R1, R2 = same), which were treated with H2S to give thioamides III, which were S-methylated with MeI to give thioimidic esters IV, which were treated with NH4OAc to give title compds. V. V can be used as thrombin inhibitors; V (R = PhCH2O2C, NR1R2 = piperidino) was the most effective inhibitor.
IT **103879-80-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of)
RN 103879-80-7 CAPLUS
CN Phenylalanine, N-(N-benzoylglycyl)-4-cyano-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

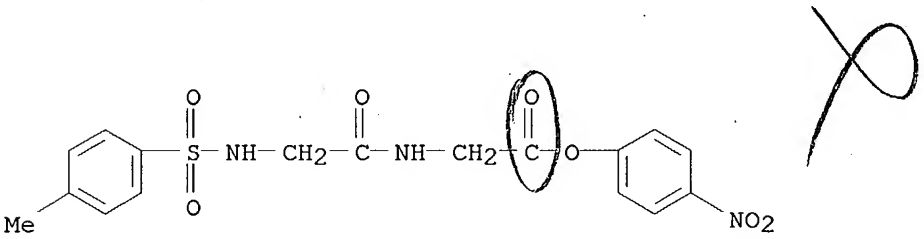


L71 ANSWER 25 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:456903 CAPLUS
DN 105:56903
TI Synthesis and kinetic parameters of hydrolysis by trypsin of some acyl-arginyl-p-nitroanilides and peptides containing arginyl-p-nitroanilide
AU Juliano, M. A.; Juliano, L.
CS Dep. Biofis., Esc. Paulista Med., Sao Paulo, 04034, Brazil
SO Brazilian Journal of Medical and Biological Research (1985), 18(4), 435-45
CODEN: BJMRDK; ISSN: 0100-879X
DT Journal
LA English
AB Four acylarginine-p-nitroanilides, 9 acetyl- (or benzoyl)aminoacylarginine-p-nitroanilides, and 12 acyl- (or free α-amino-)dipeptidylarginine-p-nitroanilides were synthesized, and the kinetic parameters for tryptic hydrolysis of these substrates were determined in 100 mM Tris-HCl buffer, pH 8.0, containing 10 mM CaCl2 at 37°. Among the acylarginine-p-nitroanilides, octanoylarginine-p-nitroanilide was hydrolyzed 4-fold more rapidly by trypsin than the commonly used substrate, benzoylarginine-p-nitroanilide. The best trypsin substrates contained proline and norleucine at subsite P2, indicating that unbranched aliphatic side-chain folded, as the β, γ, and δ methylenes are in proline, provides the most favorable conditions for S2P2 interaction. Extending the length of the substrates from di- to tripeptidyl-p-nitroanilide did not have a large influence on the kinetic parameters. However, phenylalanine at the P3 position had a clearly favorable effect, in contrast to proline, which was unfavorable only when the benzoyl group was present at P4. The series, Ac-Phe-(or D-Phe)-Gly-Arg-p-nitroanilide and Phe-(or D-Phe)-Gly-Arg-p-nitroanilide were studied. The benzyl side-chain of D-phenylalanine had a more favorable interaction at S3 than phenylalanine. A P4-CO...HN-S4 H-bond was proposed to stabilize the P3/S3 interaction when an Ac group was present on the α-NH2 group of the phenylalanine residue, and the reverse would be expected to occur for the corresponding D-epimer.
IT **103418-67-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reaction kinetics with trypsin)
RN 103418-67-3 CAPLUS
CN L-Argininamide, N-benzoylglycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

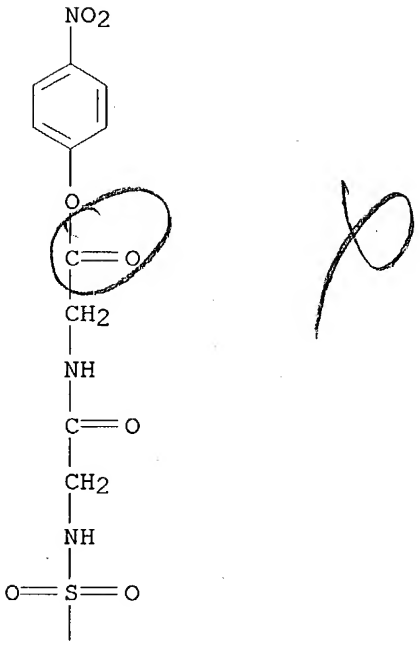


L71 ANSWER 26 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1985:25017 CAPLUS
DN 102:25017
TI Synthesis of Nα-(arylsulfonylglycylglycyl)-4-amidinophenylalanine amides as thrombin inhibitors
AU Voigt, B.; Wagner, G.
CS Sekt. Biowiss., Karl-Marx-Univ., Leipzig, Ger. Dem. Rep.
SO Pharmazie (1984), 39(6), 379-81
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
AB The title compds. I (R = piperidine, pyrrolidino, morpholino, BuNH; R1 = p-tolyl, α-naphthyl, β-naphthyl) were prepared as thrombin inhibitors. Aminolysis of 4-R1SO2NHCH2CONHCH2COR2 (II, R2 = 4-O2NC6H4O) with 4-NCC6H4CH2CH(NH2)CO2H.HCl gave II [R2 = NHCH(CO2R3)CH2C6H4R4-4] (III, R3 = H, R4 = cyano), which were esterified to give III (R3 = OC6H4NO2-4, R4 = cyano) and the product treated with amines to give III (R3 = R, R4 = cyano). H2S treatment gave III (R3 = R, R4 = CSNH2) which were methylated to III [R3 = R, R4 = C(SMe):NH].HI and the products treated with NH4OAc in MeOH to give I.HI. The (arylsulfonyl)glycylglycine group gave decreased thrombin inhibitory activity.
IT **93886-72-7P 93886-73-8P 93909-49-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aminolysis of, with cyanophenylalanine)
RN 93886-72-7 CAPLUS
CN Glycine, N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

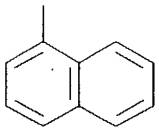


RN 93886-73-8 CAPLUS
CN Glycine, N-[N-(1-naphthalenylsulfonyl)glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

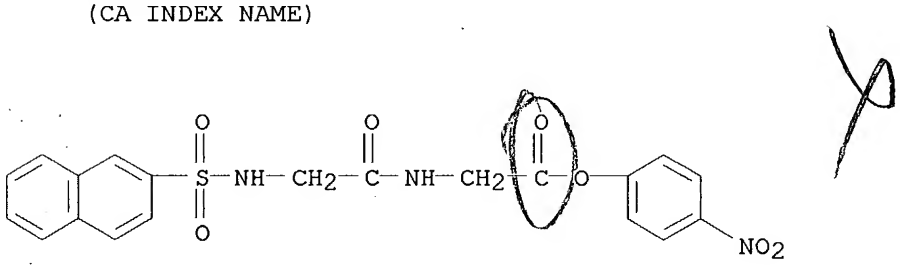
PAGE 1-A



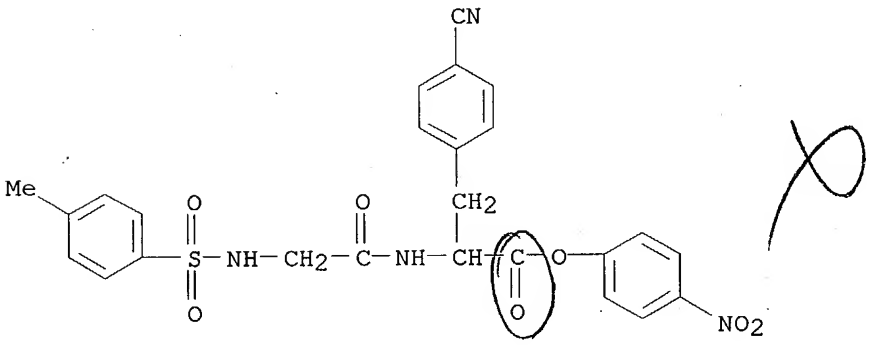
PAGE 2-A



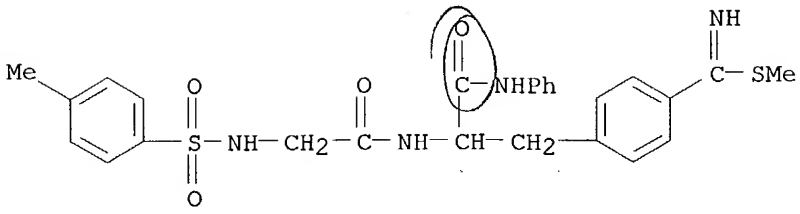
RN 93909-49-0 CAPLUS
CN Glycine, N-[N-(2-naphthalenylsulfonyl)glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



L71 ANSWER 27 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:611666 CAPLUS
DN 101:211666
TI Synthesis of Nα-(arylsulfonylglycyl)amidinophenylalaninamides as highly active inhibitors of thrombin
AU Wagner, G.; Voigt, B.; Vieweg, H.
CS Sekt. Biowiss., Karl-Marx-Univ. Leipzig, Leipzig, DDR-7010, Ger. Dem. Rep.
SO Pharmazie (1984), 39(4), 226-30
CODEN: PHARAT; ISSN: 0031-7144
DT Journal
LA German
AB The title compds. I (R = piperidino, pyrrolidino, BuNH, PhNH, morpholino; R1 = p-tolyl, α-, β-naphthyl; amidino at 3 or 4), as the HCl or HI salts, were prepared from purified cyanophenylalanines after introducing the arylsulfonylglycyl group, activating the CO2H group by forming the 4-O2NC6H4 ester, subsequent aminolysis, and conversion of the cyano into an amidino function. Addnl., several esters and an acid with the basic structure of I were prepared I (R = piperidino, R1 = 2-naphthyl, 4-amidino) had the strongest antithrombin activity with Ki = 6 + 10-9 mol/L using S-2238 substrate.
IT **84792-45-0P 92740-67-5P 92771-17-0P 92771-18-1P 92771-19-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aminolysis of)
RN 84792-45-0 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

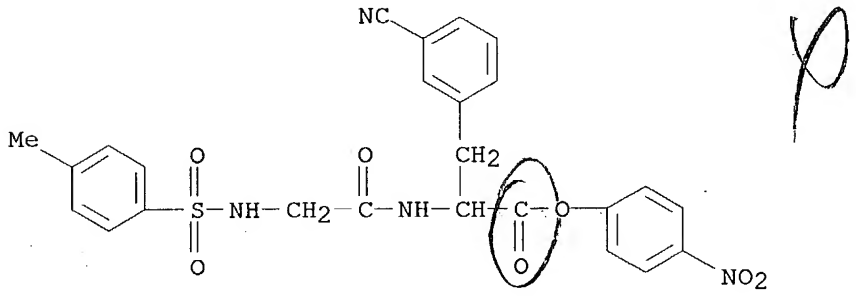


RN 92740-67-5 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-[imino(methylthio)methyl]-N-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



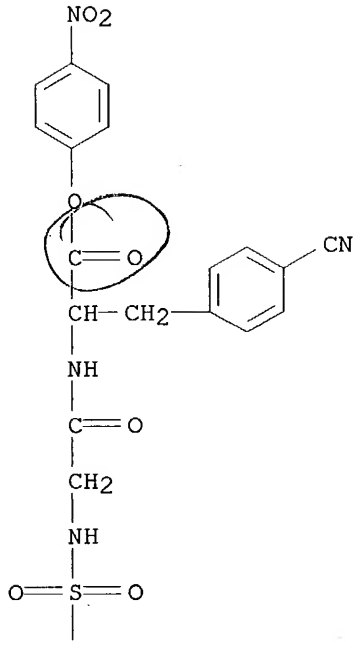
● HI

RN 92771-17-0 CAPLUS
CN Phenylalanine, 3-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

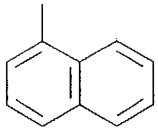


RN 92771-18-1 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-(1-naphthalenylsulfonyl)glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

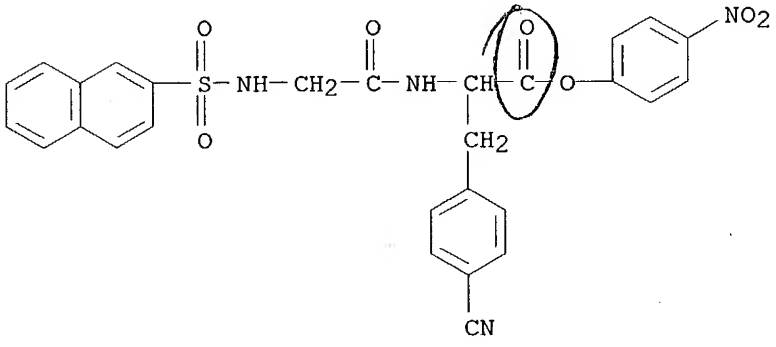
PAGE 1-A



PAGE 2-A



RN 92771-19-2 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-(2-naphthalenylsulfonyl)glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

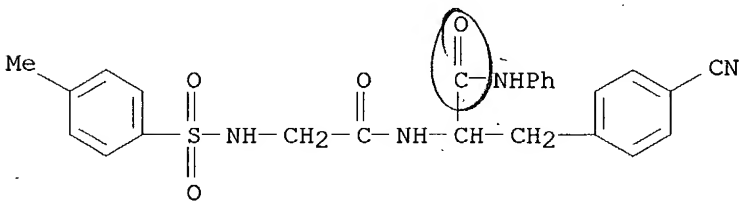


IT **92771-23-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrosulfuration of)

RN 92771-23-8 CAPLUS

CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-cyano-N-phenyl- (9CI) (CA INDEX NAME)

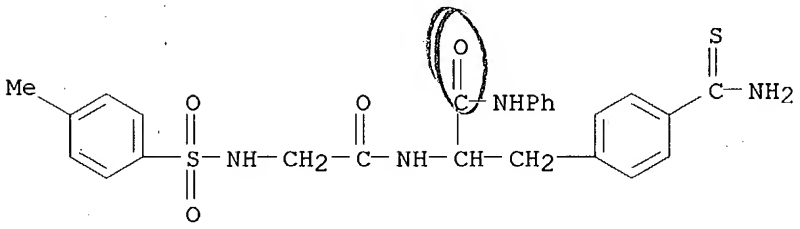


IT **92771-14-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and S-methylation of)

RN 92771-14-7 CAPLUS

CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminothioxomethyl)-N-phenyl- (9CI) (CA INDEX NAME)

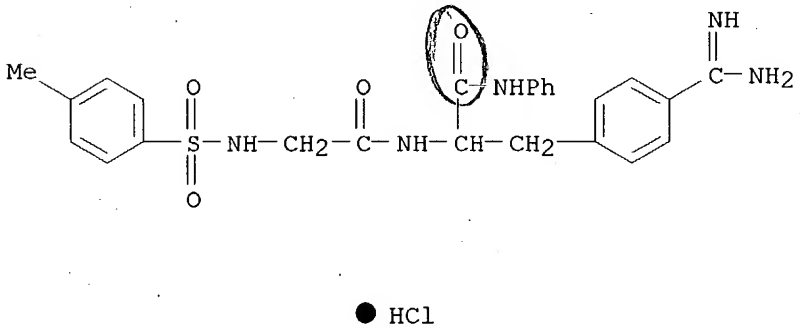


IT **92842-14-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as thrombin inhibitor)

RN 92842-14-3 CAPLUS

CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminoiminomethyl)-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

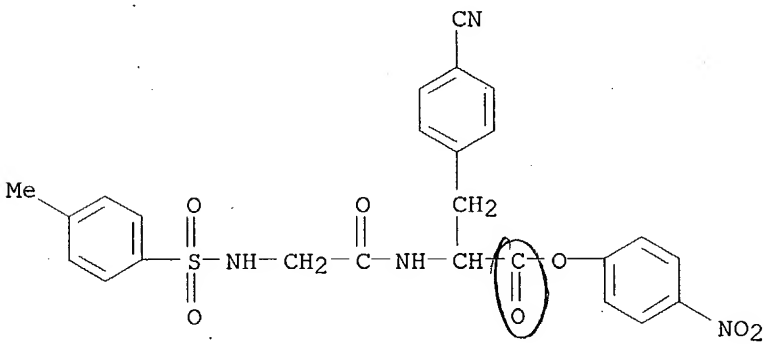


● HCl

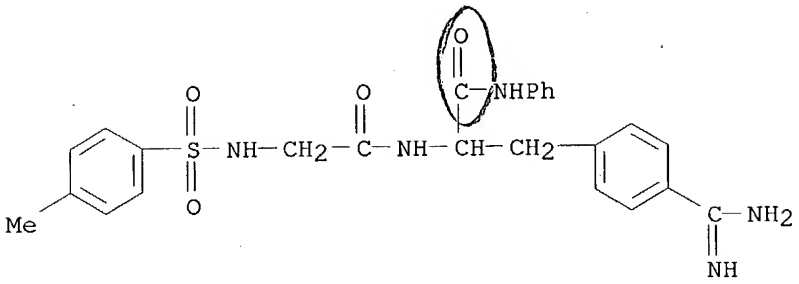
L71 ANSWER 28 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:107770 CAPLUS
DN 98:107770
TI Nα-Aryl- or Nα-heteroarylsulfonyl aminoacylated amidinophenylalanine amides
IN Wagner, Guenther; Voigt, Bernd; Vieweg, Helmut; Markwardt, Fritz; Stuerzebecher, Joerg
PA Ger. Dem. Rep.
SO Ger. (East), 17 pp.
CODEN: GEXXA8
DT Patent
LA German
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DD 155954	Z	19820721	DD 1981-227387	19810203
DD 155954	B1	19881109		
PRAI DD 1981-227387		19810203		

OS CASREACT 98:107770
AB Title compds. I (R = aryl, heteroaryl; R1 = H, alkyl, aryl, aralkyl; R2 = alkyl, aryl, aralkyl; NR1R2 = heteroaliph. ring; n = 1-5; amidino group at m- or p-position) were prepared as thrombin inhibitors for use as anticoagulants (no data). Thus, Tos-Gly-Cl (Tos = tosyl) was coupled with 3- and 4-cyanophenylalanine-HCl in 1N NaOH to give peptide II and its p-isomer, which were esterified with HOC6H4NO2-4 by DCC to give the p-nitrophenyl esters, which were treated with piperidine to give piperidides III (R3 = m-CN, p-CN). The latter were treated with H2S to give the thioamides, which were treated with MeI and then with NH4OAc/MeOH to give III [R3 = m-C(:NH)NH2, p-C(:NH)NH2].
IT **84792-45-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with piperidine)
RN 84792-45-0 CAPLUS
CN Phenylalanine, 4-cyano-N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



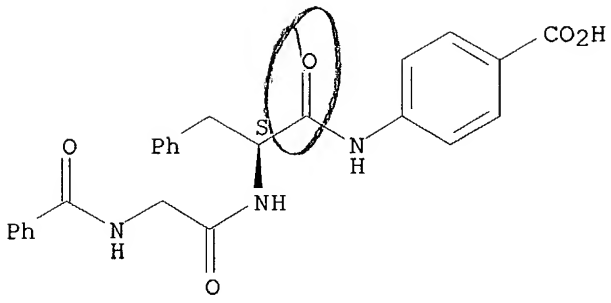
IT **84792-59-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 84792-59-6 CAPLUS
CN Phenylalaninamide, N-[(4-methylphenyl)sulfonyl]glycyl-4-(aminoiminomethyl)-N-phenyl-, monohydriodide (9CI) (CA INDEX NAME)



● HI

L71 ANSWER 29 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:67751 CAPLUS
DN 98:67751
TI Membrane-bound kidney neutral metalloendopeptidase: interaction with synthetic substrates, natural peptides, and inhibitors
AU Almenoff, June; Orlowski, Marian
CS Mt. Sinai Sch. Med., City Univ. New York, NY, 10029, USA
SO Biochemistry (1983), 22(3), 590-9
CODEN: BICHAW; ISSN: 0006-2960
DT Journal
LA English
AB A neutral metalloendopeptidase with thermolysin-like specificity was purified to apparent homogeneity from the particulate fraction of rabbit kidney homogenates. After preparation of a deoxycholate extract, the enzyme was released from membranes by papain treatment and separated from other membrane-bound enzymes including dipeptidyl aminopeptidase IV, aminopeptidase M, and γ-glutamyl transpeptidase by chromatog. on Sephadex G-200, phenyl-Sepharose, and CM-cellulose columns. The isolated enzyme had a mol. weight of .apprx.95,000 and was inhibited by thiols, metal chelators, phosphoramidon, and thiorphan. It was apparently identical with kidney neutral metalloendopeptidase and similar to bovine pituitary metalloendopeptidase and to an enzyme designated as enkephalinase. Studies with a series of synthetic substrates showed that the enzyme preferentially cleaved bonds in which the amino group was provided by a hydrophobic amino acid residue. Several biol. active peptides, such as methionine- and leucine-enkephalin, dynorphin, bradykinin, and angiotensin I, were degraded by cleavage of the same type of bond. The endopeptidase acted as a dipeptidyl carboxypeptidase on peptides having a hydrophobic residue in the penultimate position. N-[1(RS)-Carboxy-2-phenylethyl] derivs. of phenylalanyl- and alanyl-p-aminobenzoate were synthesized and tested as potential inhibitors. The two diastereomers of N-[1(R,S)-carboxy-2-phenylethyl]phenylalanyl-p-aminobenzoate were separated by high-pressure liquid chromatog.; the more potent isomer had a Ki of 2.9 + 10-8 M. The inhibitory potency of the alanyl derivs. was lower by almost 2 orders of magnitude. The data indicated that, as with thermolysin, a hydrophobic residue in the P1' position and the carboxylate group complexing with the active-site Zn accounted for the inhibitory action of these derivs.
IT **84041-48-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and metalloendopeptidase of kidney inhibition by)
RN 84041-48-5 CAPLUS
CN L-Phenylalaninamide, N-benzoylglycyl-N-(4-carboxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.


CO2H
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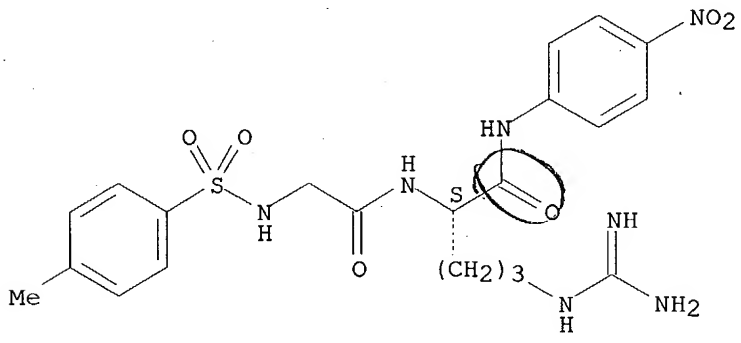
S
Ph
N
H
O
NH
Ph
N
H
O

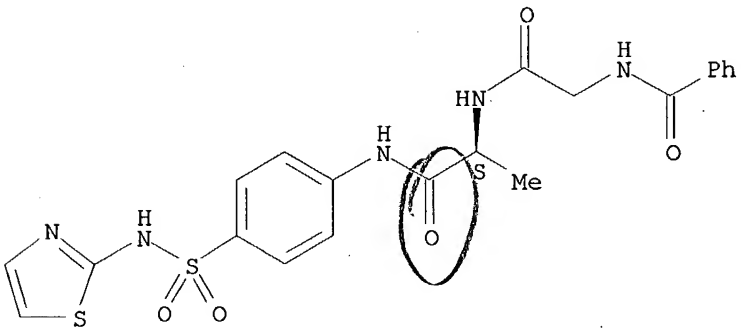
L71 ANSWER 30 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:49235 CAPLUS
DN 98:49235
TI Two automated methods for plasma antithrombin III compared, and the clinical significance of the results
AU Prellwitz, Winfried; Schmitt, Karl Friedrich; Machner, Mathias; Schuster, Carl Johannes; Weilemann, Ludwig
CS Dep. Clin. Chem., Univ. Mainz, Mainz, D 6500, Fed. Rep. Ger.
SO Clinical Chemistry (Washington, DC, United States) (1982), 28(11), 2249-53
CODEN: CLCHAU; ISSN: 0009-9147
DT Journal
LA English
AB Antithrombin III (AT III) activity was determined with 2 different new chromogenic substances [Chromozym-TH (tosyl-Gly-Arg-p-nitroanilide) and α-N-carbobenzyloxy-L-lysine-thiobenzyl ester] with both a discrete (aca) and a centrifugal analyzer (COBAS BIO). The correlation between the Chromozym-TH/centrifugal analyzer and Du Pont ester/aca methods was good. Precision within and between runs was similar to that for typical enzymic detns. AT III in plasma of healthy men and women ranged 76.6-141.1% (100% = normal). No significant differences ascribable to oral contraceptives were found. AT III activity was decreased in 27% of patients with acute thromboembolic diseases, in 48% of patients the 1st day after abdominal operations without complications, and in 100% of patients with reversible or irreversible shock. In patients receiving continuous therapy with heparin (1500 USP units/h), no decrease in AT III within 96 h of beginning treatment was observed Plasma from 14 of 16 patients with disseminated intravascular coagulopathy showed a decrease in AT III of 17-51% of normal before and during heparin therapy. All 16 patients were treated with AT III concentrate During such treatment, AT III in plasma must be monitored over short intervals to assure that sufficiently high proportions of AT III (>70% of normal) are reached.
IT **84213-42-3**
RL: BIOL (Biological study)
(in antithrombin III determination, in blood plasma of humans)
RN 84213-42-3 CAPLUS
CN L-Argininamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



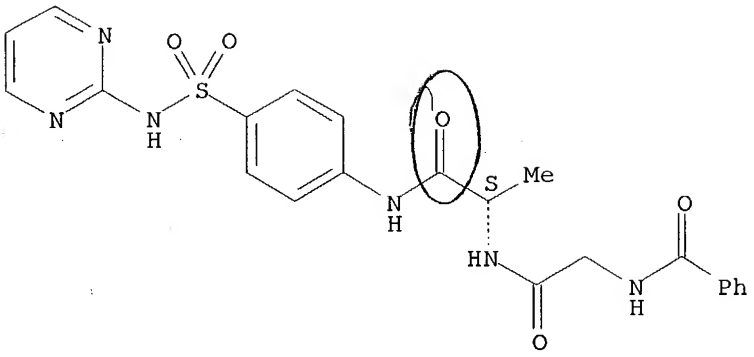
L71 ANSWER 31 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:439805 CAPLUS
DN 87:39805
TI Synthesis of some N4-(amino acid or dipeptide)-sulfanilamide derivatives
AU El-Naggar, A. M.; Zaher, M. R.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Roczniki Chemii (1976), 50(12), 2187-91
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English
AB 4-RNHC6H4SO2NHR1 [I; R = Bz-Gly, R1 = H, R2, R3, C(:NH)NH2; R = Tos-β-Ala, R1 = R2, C(:NH)NH2; where Tos = 4-MeC6H4SO2] were prepared by condensing R-NHNH, with the appropriate 4-H2NC6H4SO2NHR1 (II) by azide couplings. I (R = phthaloylglycyl, phthaloyl-β-alanyl, R1 = H, R3; R = Tos-β-Ala, Tos-Ala, R1 = R3) were prepared by acylating the appropriate II with the appropriate R-Cl. Bz-Gly-NHNH2 was coupled to H-X-OMe (X = Ala, Val) to give Bz-Gly-X-OMe which were treated with NH2NH2 to give Bz-Gly-X-NHNH2 (III). Bz-Gly-X-NHC6H4SO2NHR1 (IV; X = Ala, R1 = R2, R3; X = Val, R1 = R3) were prepared by coupling III to the appropriate II. I (X = Tos-β-Ala, Tos-Ala; R1 = R3) possess antibacterial against Bacillus subtilis and Escherichia coli, but they were inactive against Micrococcus pyogenes and several other bacteria. IV (X = Ala, R1 = R2) was active against B. subtilis and inactive against all other microorganisms tested.
IT **63203-26-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antibacterial activity of)
RN 63203-26-9 CAPLUS
CN L-Alaninamide, N-benzoylglycyl-N-[4-[(2-thiazolylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



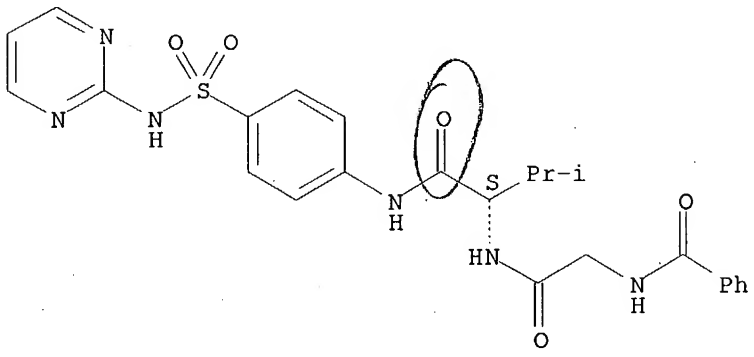
IT **63203-25-8P 63203-27-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63203-25-8 CAPLUS
CN L-Alaninamide, N-benzoylglycyl-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



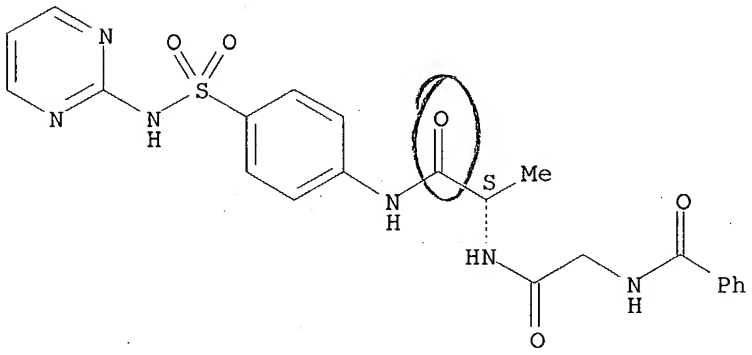
RN 63203-27-0 CAPLUS
CN L-Valinamide, (N-benzoylglycyl)-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



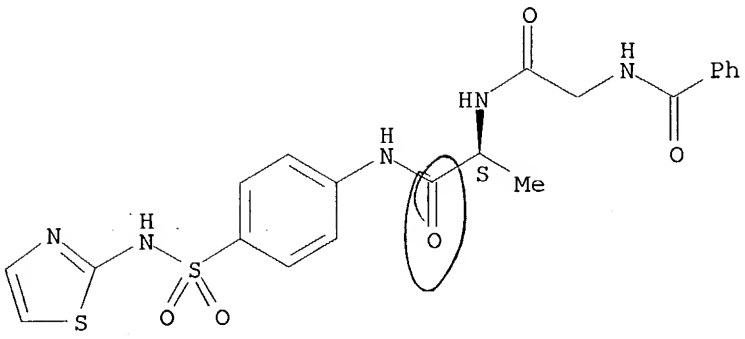
L71 ANSWER 32 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:433009 CAPLUS
DN 87:33009
TI Metal complexes and biological activities of some peptides containing glycine, alanine, and hippuric acid
AU El-Naggar, A. M.; Shehata, Y. A.; Zaher, M. R.
CS Fac. Sci., Al-Azhar Univ., Cairo, Egypt
SO Roczniki Chemii (1977), 51(2), 233-7
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English
AB Spectrophotometric studies were carried out on the formation of Cu, Fe, and Ni complexes with di- and tripeptides containing glycine, alanine, and hippuric acid. Replacement of the end amino acid in the peptide by 2-aminopyridine, sulfadiazine, sulfathiazole, sulfanilamide, sulfaguanidine, urea, or β-alanine gave compds. which did not form the normal complexes with Cu2+, Fe3+, and Ni2+ ions. The hydrazides of the peptides participated in the usual way in the formation of complexes. Some of the obtained complexes exhibited distinct antibacterial activity.
IT **63203-25-8DP**, copper complexes **63203-26-9DP**, copper complexes **63203-27-0DP**, copper complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63203-25-8 CAPLUS
CN L-Alaninamide, N-benzoylglycyl-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



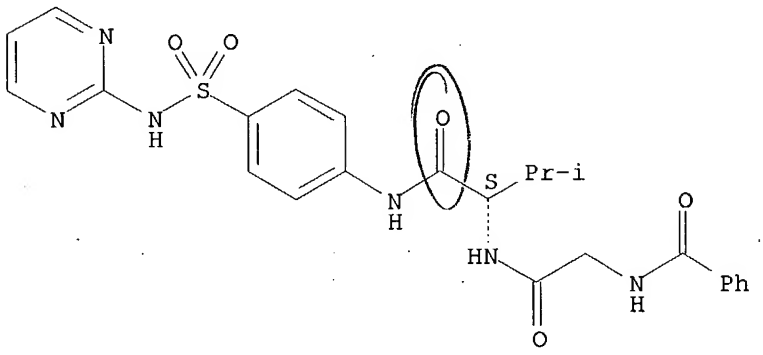
RN 63203-26-9 CAPLUS
CN L-Alaninamide, N-benzoylglycyl-N-[4-[(2-thiazolylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



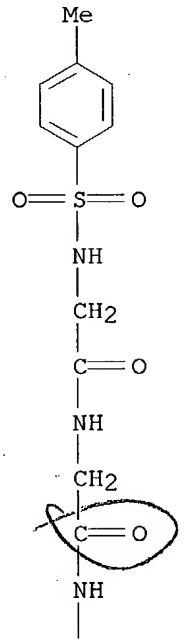
RN 63203-27-0 CAPLUS
CN L-Valinamide, (N-benzoylglycyl)-N-[4-[(2-pyrimidinylamino)sulfonyl]phenyl]- (9CI) (CA INDEX NAME)

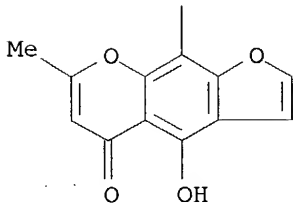
Absolute stereochemistry.



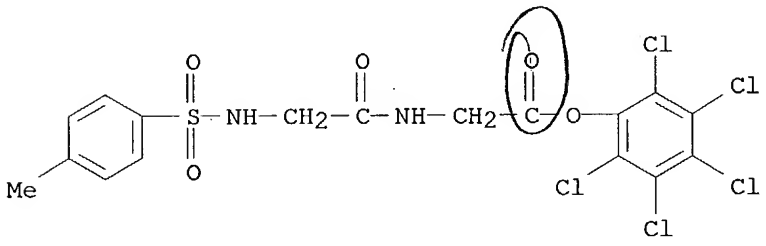
L71 ANSWER 33 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:73090 CAPLUS
DN 86:73090
TI Synthesis of some protected amino acid and dipeptide derivatives of desmethylvisnagin
AU Elgamal, M. H. A.; El-Naggar, A. M.; El-Tawii, B. A. H.; Abd El-Salam, A. M.
CS Natl. Res. Cent., Cairo, Egypt
SO Roczniki Chemii (1976), 50(4), 765-8
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA English
AB Aminodemethylvisnagins (I; R1 = phthaloyl, p-MeC6H4SO2; X = Gly, Ala, β-Ala, Val, Leu, D-Phe, Ser; R1 = p-MeC6H4SO2, X = Ala-Gly, Gly-Gly) were prepared by acylating II with R-X-Cl. II was prepd by reducing III with Zn in EtOH. I did not have microbiol. activity (no data).
IT **61635-38-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 61635-38-9 CAPLUS
CN Glycinamide, N-[(4-methylphenyl)sulfonyl]glycyl-N-(4-hydroxy-7-methyl-5-oxo-5H-furo[3,2-g][1]benzopyran-9-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A




Me
O
O
O
OH

L71 ANSWER 34 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:44621 CAPLUS
DN 84:44621
TI Synthesis of tertiary amines by selective diborane reduction
AU Russ, Pamela A.; Caress, Edward A.
CS Dep. Chem., George Washington Univ., Washington, DC, USA
SO Journal of Organic Chemistry (1976), 41(1), 149-51
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 84:44621
AB N-ethyl-N-(2-tosylaminoethyl)glycine hydrochloride was prepared by protecting the amine and carboxyl functions of glycylglycine with tosyl and pentachlorophenyl groups, resp., and then selectively reducing the amide carbonyl with diborane to give N-(2-tosylaminoethyl)glycine pentachlorophenyl ester (II). Acetylation of II followed by selective amide reduction with diborane and hydrolysis gave N-ethyl-N-(2-tosylaminoethyl)glycine.
IT **57066-12-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diborane reduction of)
RN 57066-12-3 CAPLUS
CN Glycine, N-[N-[(4-methylphenyl)sulfonyl]glycyl]-, pentachlorophenyl ester (9CI) (CA INDEX NAME)



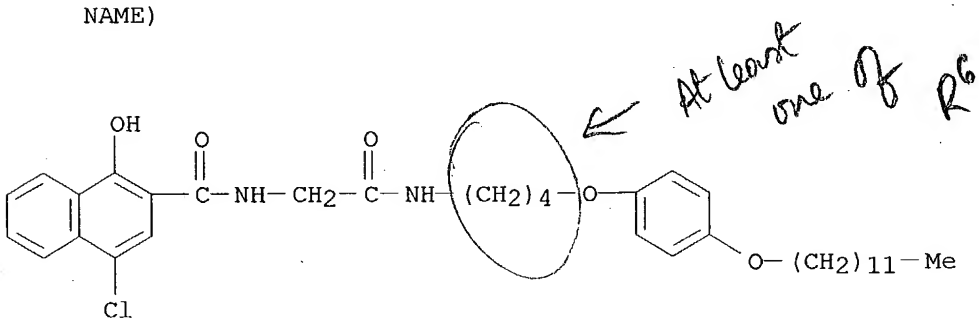
L71 ANSWER 35 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:586299 CAPLUS
DN 83:186299
TI Light-sensitive color photographic material with diffusion-resistant cyan color couplers
IN Credner, Hans H.
PA Agfa-Gevaert, Fed. Rep. Ger.
SO Ger. Offen., 18 pp. Addn. to Ger. Offen. 2,325,461.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2349562	A1	19750410	DE 1973-2349562	19731003
	GB 1469696	A	19770406	GB 1974-21738	19740516
	FR 2229998	A1	19741213	FR 1974-17377	19740517
	FR 2229998	B1	19780929		
	IT 1013190	A	19770330	IT 1974-51067	19740517
	CH 600387	A	19780615	CH 1974-6842	19740517
	JP 50020723	A2	19750305	JP 1974-55025	19740518
PRAI	DE 1973-2325461		19730519		
	DE 1973-2349562		19731003		

AB Naphtholic and phenolic light-stable, diffusion-resistant, cyan couplers for color photog. are described. Especially useful are 1-hydroxy-2-[δ-(4-dodecyloxyphenoxy)butyl]naphthamide (I), 1-hydroxy-2-[δ-(4-dodecyloxyphenoxy)butyl]-4-chloro-naphthoylglycinamide, 2-[δ-(4-dodecyloxyphenoxy)propionamido]-4,6-dichloro-5-methylphenol. Thus, I (prepared by heating δ-(4-dodecyloxyphenoxy)butylamine with Ph 1-hydroxy-2-naphthoate for 3 hr at 130°) 2.1 g in EtOAc 10 ml was added to a 5% aqueous gelatin solution containing Na dodecylsulfonate 0.4 g, emulsified, added to a gelatin-Ag halide emulsion containing 0.024 moles Ag halide, coated on a cellulose acetate support, exposed through a cyan step wedge, developed in a developer containing N,N-diethyl-p-phenylenediamine, and then exposed to a fluorescent lamp (7.5 + 106 lx-sec) to give at a d. of 0.5 a 12% decrease in d. and at a d. of 1.5 a 6% decrease in d. vs. 26 and 8, resp., for a control containing 1-hydroxy-2-[δ-(2,4-di-tert-amylphenoxy)butyl]naphthamide.

IT **57249-77-1**
RL: TEM (Technical or engineered material use); USES (Uses)
(photog. cyan coupler)

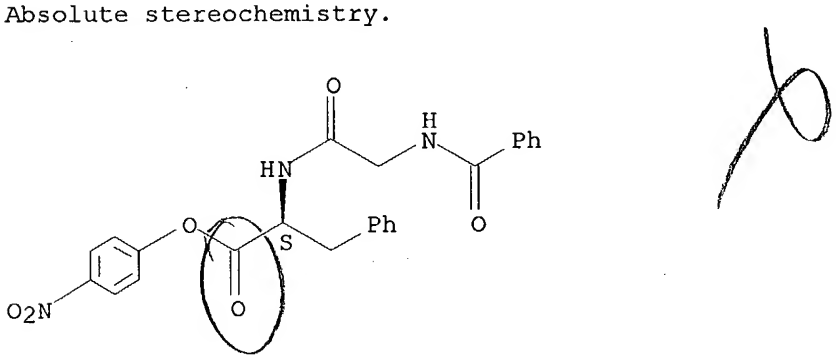
RN 57249-77-1 CAPLUS
CN 2-Naphthalenecarboxamide, 4-chloro-N-[2-[[4-[4-(dodecyloxy)phenoxy]butyl]amino]-2-oxoethyl]-1-hydroxy- (9CI) (CA INDEX NAME)



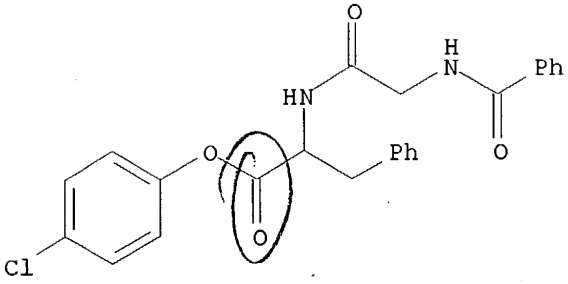
At least one of R6 & R3 is not H.

L71 ANSWER 36 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1967:105183 CAPLUS
DN 66:105183
TI Amino acids and peptides. XXV. The mechanism of the base-catalyzed racemization of the p-nitrophenyl esters of acylpeptides
AU Antonovics, Ieva; Young, Geoffrey Tyndale
CS Oxford Univ., Oxford, UK
SO Journal of the Chemical Society [Section] C: Organic (1967), (7), 595-601
CODEN: JSOOAX; ISSN: 0022-4952
DT Journal
LA English
AB cf. CA 64, 5200f. The p-nitrophenyl esters of benzoyl- and benzyloxycarbonyl glycyl-L-phenylalanine (I) are racemized by Et3N in CH2Cl2 much more rapidly than are the analogous esters of benzyloxycarbonyl- and phthaloyl-L-phenylalanine. The acyldipeptide esters react reversibly with Et3N to give the corresponding oxazolone, the equilibrium being greatly in favor of the ester. The racemization of benzoylglycyl-L-phenylalanine p-nitrophenyl ester by Et3N is suppressed by the addition of a large excess of the oxazolone derived from benzyloxycarbonylglycylphenylalanine, which reacts immediately with the p-nitro-phenoxide anion and so prevents the back-reaction by which racemic ester is formed. This experiment distinguishes clearly between the direct exchange mechanism of racemization and that through the oxazolone. Such racemization proceeds through the intermediate formation, racemization, and coupling of the corresponding oxazolone. Evidence is also given that the conversion of I into its p-nitrophenyl ester by means of diphenylketene is accompanied by racemization. 23 references.
IT **2900-37-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and racemization of)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

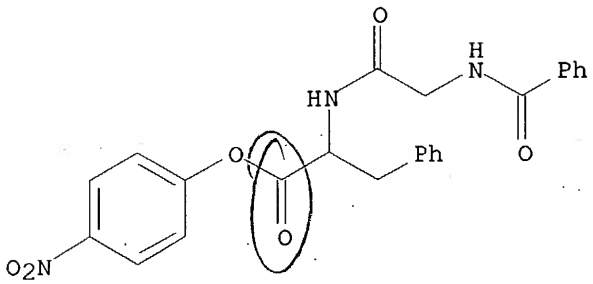
Absolute stereochemistry.



IT **13716-78-4P 13716-80-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13716-78-4 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-chlorophenyl ester, DL- (8CI) (CA INDEX NAME)

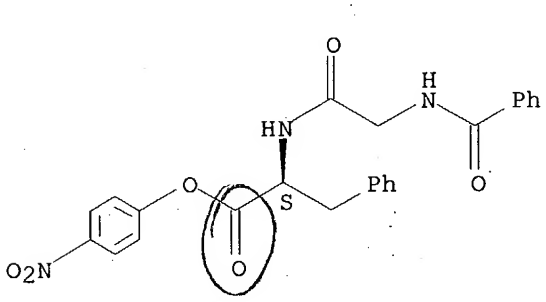


RN 13716-80-8 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, DL- (8CI) (CA INDEX NAME)



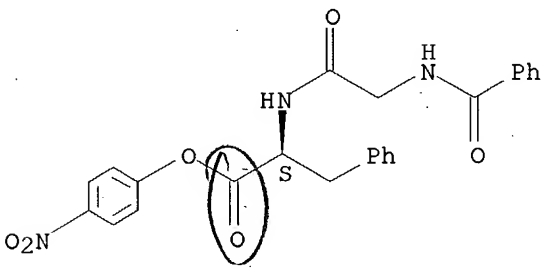
L71 ANSWER 37 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1965:489240 CAPLUS
DN 63:89240
OREF 63:16450d-f
TI Contribution to the discussion on racemization
AU Young, G. T.; Antonovics, I.
SO Acta Chimica Academiae Scientiarum Hungaricae (1965), 44(1-2), 43-4
CODEN: ACASA2; ISSN: 0001-5407
DT Journal
LA English
AB cf. preceding abstract When benzoylglycyl-L-phenylalanine p-nitrophenyl ester in tetrahydrofuran was treated with one equivalent of Et3N the optical rotation fell very much more rapidly than when the benzyloxycarbonyl(CBZ)-L-phenylalanine ester was similarly treated, and when CH2Cl2 was used as solvent, benzoylglycyl-DL-phenylalanine p-nitrophenyl ester separated out within 1 hr. at room temperature However, the ir absorption of the solution showed only a very small peak at 1830 cm.-1 (oxazolone C:O), and the same observation was made with the CBZ analog. Addition of 1 equivalent each of Et3N and p-nitrophenol to the oxazolones very rapidly extinguished the 1830 cm.-1 peak. Equimolar amts. of CBZ-L-phenylalanine p-nitrophenyl ester and of the oxazolone derived from benzoylglycyl-L-phenylalanine in CH2Cl2 were treated with one equivalent of Et3N 1 hr. at room temperature The p-nitrophenyl ester was recovered. Chromatography showed the presence of the p-nitrophenyl esters of both the CBZ-and the benzoyl-dipeptide esters, and the latter ester was isolated (as racemate). This evidence is viewed as consistent with racemization proceeding through the oxazolone formed rapidly but being present in only small concentration
IT **2900-37-0**, Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L-
(coupling reactions of, racemization in relation to)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L71 ANSWER 38 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1965:480972 CAPLUS
DN 63:80972
OREF 63:14976g-h
TI The mechanism of racemization during the coupling of acyl peptides
AU Antonovics, I.; Young, G. T.
CS Univ. Oxford, UK
SO Chemical Communications (London) (1965), (17), 398-9
CODEN: CCOMA8; ISSN: 0009-241X
DT Journal
LA English
AB When a solution of benzoyl-L-leucine p-nitrophenyl ester in dichloromethane was treated with one molar proportion of triethylamine, the optical rotation decreased by 50% in 50 min. at room temperature -far more rapidly than with phthaloyl-L-phenylalanine p-nitrophenyl ester (.apprx. 5% in the same time). It was concluded that the racemization followed chiefly, if not exclusively, through the oxazolone.
IT **2900-37-0**, Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (coupling and racemization of)
RN 2900-37-0 CAPLUS
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



L71 ANSWER 39 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:31703 CAPLUS
DN 56:31703
OREF 56:6084e-i,6085a-i,6086a-f
TI Insulin peptides. I. Synthesis of cysteine-containing peptides related to the A-chain of sheep insulin
AU Katsoyannis, Panayotis G.
CS Univ. of Pittsburgh, Pittsburgh, PA
SO Journal of the American Chemical Society (1961), 83, 4053-7
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
OS CASREACT 56:31703
AB Several protected cysteine-containing peptides with amino acid sequences found in the intra-chain ring region of the A-chain of sheep insulin were synthesized. For the protection of the SH functions of these peptides, the p-nitrobenzyl, carbobenzyloxy, and benzylthiomethyl groups, which can be removed selectively, were employed. Evidence is presented that the S-benzyl-thiomethyl-L-cysteine (I) does not remain intact on treatment with HBr in AcOH, contrary to a previous report by Pimlott and Young (CA 53, 9082f). S-p-Nitrobenzyl-L-cysteine (II) (15.2 g.) in 20 cc. cold H2O and 60 cc. N NaOH treated in portions with stirring with 12.8 cc. ClCO2CH2Ph and 80 cc. N NaOH during 0.5 hr., stirred 0.5 hr. at room temperature, washed with Et2O, acidified with HCl, and extracted with EtOAc yielded 23 g. oily N-carbobenzyloxy derivative (III) of II. III in Et2O with cyclohexylamine in Et2O gave the cyclohexylamine salt of III, needles, m. 129-30° (EtOH-Et2O) (all m.ps. are corrected), [α]28D -2.2° (c 1, EtOH). L-Alanine Me ester-HCl (4.2 g.) in 50 cc. tetrahydrofuran (THF) stirred 20 min. with 4.1 cc. Et3N, cooled, filtered, treated with 11 g. III and 6.2 g. N,N'-dicyclohexylcarbodiimide (IV) in 50 cc. THF, kept at 0° overnight, filtered from the N,N'-dicyclohexylurea (V), the THF replaced by 600 cc. EtOAc, and the solution worked up gave 8.95 g. Me ester (VI) of N-carbobenzyloxy-S-p-nitrobenzyl-L-cysteinyl-L-alanine (VII), m. 173-4°, [α]28D -39.6° (c 1.5, HCONMe2). VI (4.75 g.) in 50 cc. dioxane and 50 cc. Me2CO treated with stirring during 0.5 hr. with 11 cc. N NaOH, stirred 45 min. at room temperature, diluted with 150 cc. cold H2O, and acidified with 6N HCl gave 3.65 g. VII, m. 157-9° (50% aqueous EtOH), [α]28D -45.5° (c 1, HCONMe2). VII (6.93 g.) and 2.1 cc. Et3N in 70 cc. THF treated at -5° with 2 cc. ClCO2CH2CHMe2 (VIII) and after 10 min. with Et glycinate (from 3.5 g. HCl salt and dry NH3) in 25 cc. THF, kept 10 min. at -5° and 45 min. at room temperature, and worked up gave 7 g. N-carbobenzyloxy-S-p-nitrobenzyl-L-cysteinyl-L-alanylglycine Et ester (IX), needles, m. 212° (60% aqueous AcOH), [α]28D -25.4° (c 1, HCONMe2). Carbobenzyloxyglycine (8.20 g.) in 50 cc. THF containing 5. cc. Et3N treated at -5° with 5.28 cc. VIII and after 10 min. with valine Me ester (from 6.8 g. HCl salt in 80 cc. THF and 5.6 cc. Et3N), stirred 15 min. at -5° and 1 hr. at room temperature, and evaporated to dryness in vacuo, and the residue dissolved in 150 cc. EtOAc and 50 cc. H2O, and the organic layer worked up gave 8.5 g. N-carbobenzyloxyglycyl-L-valine Me ester (X), m. 78° [α]28D -15.5° (c 1.5, EtOH). IX (2.21 g.) in 4 cc. AcOH treated 1 hr. at room temperature with 10 cc. 4N HBr-AcOH, concentrated to 1/3 volume in vacuo, diluted with 100 cc. dry Et2O, and filtered, the residue washed, dried, suspended in 10 cc. THF and 0.87 cc. Et3N, stirred 10 min., and filtered, the

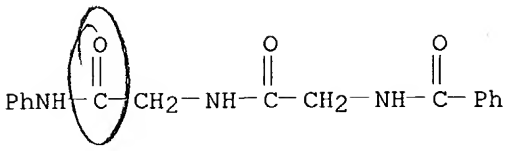
filtrate added to 2.9 g. VII and 0.86 g. Et3N in 20 cc. THF which was previously treated at -5° with 0.82 cc. VIII, the mixture stirred 15 min. at -5° and 1 hr. at room temperature, and evaporated gave 2.60 g. N-carbobenzyloxy-S-p-nitrobenzyl-L-cysteinyl-L-alanylglycyl-L-valine Me ester (XI), needles, m. 200° (50% aqueous AcOH), [α]28D -18° (c 1, HCONMe2). VII (6 g.) in 40 cc. 2N HBr stirred 1 hr. at room temperature, concentrated in vacuo, dissolved in 15 cc. MeOH, and evaporated, the residual HBr salt, m. 126-8° dissolved in 50 cc. THF and 1.65 cc. Et3N, stirred 15 min., cooled, filtered, added to 4.6 g. N,S-dicarbobenzyloxy-L-cysteine in 20 cc. tetrahydrofuran and 2.7 g. IV, kept 1 hr. at 0° and 16 hrs. at room temperature, treated with a few drops AcOH, filtered from V, and evaporated gave 6.4 g. N,S-dicarbobenzyloxy-L-cysteinyl-S-p-nitrobenzyl-L-cysteinyl-L-alanine Me ester, m. 173-4° (60% aqueous AcOH), [α]28D -54° (c 1, HCONMe2). Powdered L-Cysteine-HCl (50 g.) in 70 cc. MeOH and 58 g. PhCH2SCH2Cl refluxed 0.5 hr., concentrated in vacuo, stirred 2 hrs. at room temperature with 150 cc. dioxane and 60 cc. H2O while maintaining pH about 9 by the dropwise addition of 4N NaOH, diluted with 500 cc. H2O washed with Et2O, acidified with dilute HCl to pH 5.5, cooled several hrs., and filtered, and the residue suspended in 1.5 cc. boiling H2O, dissolved with 6N HCl, treated with Norite, adjusted with dilute NH4OH to pH 5.5, and filtered gave 45 g. I, m. 200° I (200 mg.) added to 10 cc. 2N HBr-AcOH, concentrated after 45 min. to a small volume in vacuo, and diluted with Et2O gave a precipitate which chromatographed on paper gave 4 ninhydrin-pos. spots with Rf 0.19, 0.32, 0.77, and 0.87 (Partridge system). I (200 mg.) added to 6 cc. 4N HBr-AcOH, 3 cc. (EtO)2P(O)H, and 3 cc. EtSMe and chromatographed on paper gave 1 main ninhydrin-pos. spot (Rf 0.77) and traces of 2 other ninhydrin-pos. materials, Rf 0.24 and 0.87. I (5.2 g.) in 42 cc. 98% HCO2H treated dropwise during 15 min. at 8-12° with 14 cc. Ac2O, stirred 1 hr., and diluted with 200 cc. cold H2O gave 5.2 g. N-CHO derivative (XII) of I, m. 138° (H2O), [α]27D -38.4° (c 1.24, 90% aqueous HCONMe2). X (3.3 g.) in 8 cc. AcOH and 18 cc. 4N HBr-AcOH kept 45 min. at room temperature, concentrated to half-volume in vacuo, and diluted with 300 cc. dry Et2O, the precipitate filtered off, repptd. from EtOH-Et2O, dissolved in 10 cc. HCONMe2, treated with 0.8 cc. Et3N, filtered, treated with 1.8 g. XII in 20 cc. dioxane, cooled to 0°, treated with 1.35 g. IV, kept 18 hrs. at 5°, diluted with 20 cc. HCONMe2, warmed to 45°, cooled to room temperature, acidified with AcOH, filtered from 1.38 g. V, mixed with 400 cc. H2O containing 1 cc. AcOH, and filtered yielded 2.5 g. N-formyl-S-benzylthiomethyl-L-cysteinyl-S-p-nitrobenzyl-L-cysteinyl-L-alanylglycine Et ester, m. 212-15°, [α]27D -32.1° (c 0.99, HCONMe2). X (7 g.) in 10 cc. AcOH and 25 cc. 4N HBr-AcOH kept 45 min. at room temperature, concentrated to half-volume, diluted with 400 cc. dry Et2O, and filtered, the residue dissolved in 20 cc. HCONMe2 and 60 cc. THF, treated with 1.8 cc. Et3N, filtered, concentrated to 1/4 volume, mixed with 4.7 g. N,S-dicarbo-benzyloxy-L-cysteine, cooled to 5°, treated with 2.9 g. IV in 20 cc. dioxane, kept 18 hrs. at 5°, diluted with 20 cc. dioxane, warmed to room temperature, acidified with 1 cc. AcOH, filtered from 2.8 g. V, concentrated to about 50 cc., mixed with 400 cc. 5% aqueous KHCO3, and filtered yielded 7 g. Et ester (XIII) of N,S-dicarbobenzyloxy-L-cysteinyl-S-p-nitro-benzyl-L-cysteinyl-L-alanylglycine (XIV), m. 197-8° (60% aqueous AcOH),

[α]28D -36.8° (c 1, HCONMe2). XIII (1.54 g.) in 80 cc. warm dioxane treated with 10 cc. N HCl, heated 1.5 hrs. at 60°, concentrated to 1/4 volume, and diluted with H2O gave 1.4 g. XIV.H2O, needles, m. 170-2° (60% aqueous AcOH), [α]28D -36.2° (c 1, HCONMe2). L-Leucinamide (4.6 g.) in 40 cc. HCONMe2 treated with N-carbobenzyloxy-L-serine azide (from 8.5 g. hydrazide and 2.35 g. NaNO2 in 75 cc. N HCl at 0°) in 150 cc. EtOAc, stirred 5 hrs. at 20° and 1 hr. at room temperature, diluted with 100 cc. EtOAc and 20 cc. EtOH, and worked up gave 6.6 g. N-carbobenzyloxy-L-seryl-L-leucinamide (XV), m. 181-3° (50% aqueous EtOH), [α]27D 9.1° (c 1.07, HCONMe2). S-Carbobenzyloxy-L.cysteine (12.75 g.) in 105 cc. 98% HCO2H treated dropwise at 5° during 15 min. with 42 cc. Ac2O, stirred 1 hr. at 10-15°, diluted with 350 cc. cold H2O, and filtered gave 9.8 g. N-formyl-S-carbobenzyloxy-L-cysteine (XVI), m. 141-2° (hot H2O), [α]27D -41.6° (c 1.34, HCONMe2). XV (5.25 g.) in 120 cc. EtOH containing 1.35 cc. concentrated HCl hydrogenated about 2 hrs. over 1 g. 10% Pd-C, filtered, and evaporated, the residue dried by evaporation with absolute EtOH, dissolved in 25 cc. HCONMe2, treated with 2.1 cc. Et3N, filtered, treated with 4.25 g. XVI in 20 cc. dioxane and 3.3 g. IV, stirred 20 hrs. at 5°, warmed to room temperature, acidified with AcOH, filtered from V, and worked up gave 4.2 g. N-formyl-S-carbobenzyloxy-L-cysteinyl-L-seryl-L-leucinamide, m. 219° (80% aqueous EtOH), [α]27D -13.3° (c 1.12, HCONMe2). Me ester (9.7 g.) of I.HCl in 60 cc. THF treated with 4.3 cc. Et3N, filtered, treated with 4.35 g. N-formyl-L-valine in 25 cc. THF and 6.8 g. IV, stirred 5 hrs. at 5° and 1 hr. at room temperature, acidified with a few drops AcOH, filtered from 6.9 g. V, concentrated to 15 cc., and diluted with 150 cc. H2O containing 1 cc. AcOH gave 6.8 g. Me ester (XVII) of N-formyl-L-valyl-S-benzylthiomethyl-L-cysteine (XVIII), m. 128-9° (MeOH), [α]27D -50.0° (c 1.46, HCONMe2). XVIII (1.6 g.) in 30 cc. MeOH and 8 cc. N HCl refluxed 1 hr. and evaporated, and the residue evaporated 3 times with MeOH, dissolved in 15 cc. MeOH, and diluted with 100 cc. Et2O gave 1.12 g. XVIII.HCl, m. 161-2°, [α]27D -4.9° (c 1.12, HCONMe2), Rf 0.74. N-Carbobenzyloxy-L-valine (3.8 g.) and 2.1 cc. Et3N in 30 cc. THF treated at -5° with stirring with 2 cc. VI and after 10 min. with XVIII (from XVII.HCl and 2.1 cc. Et3N) in 30 cc. THF, kept 0.5 hr. at -5° and 6 hrs. at room temperature, concentrated to 15 cc., and poured into 300 cc. H2O containing 2 cc. concentrated HCl yielded 6.3 g. N-carbobenzyloxy-L-valyl-S-benzylthiomethyl-L-cysteine Me ester (XIX), m. 112° (70% aqueous MeOH), [α]30D -28.8° (c 1.05, HCONMe2). XIX (100 mg.) added to 4 cc. 2N HBr-AcOH, kept 1 hr. at room temperature, diluted with dry Et2O, and filtered gave a precipitate which yielded 4 ninhydrin-pos. spots with Rf 0.38, 0.48, 0.60, and 0.77. XIX (100 mg.), 2 cc. 4N HBr-AcOH, 1 cc. (EtO)2P(O)H, and 1 cc. EtSMe kept 1 hr. at room temperature and worked up after 1 hr.with 1:1 EtOAc-petr. ether gave a heavy oil which showed 1 main ninhydrin-pos. component with Rf 0.76 and traces of 2 other components with Rf 0.42 and 0.54.

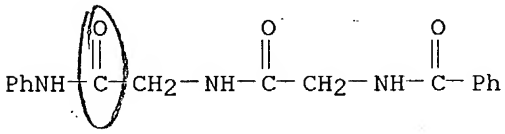
IT **93818-92-9**, Acetanilide, 2-(2-benzamidoacetamido)-
(preparation of)

RN 93818-92-9 CAPLUS

CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



L71 ANSWER 40 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1962:31702 CAPLUS
DN 56:31702
OREF 56:6084c-e
TI Reactions of formylamino acids and acyldipeptides with dicyclohexylcarbodiimide
AU Siemion, Ignacy Z.; Nowak, Kornel
CS Akad. Med., Wroclaw, Pol.
SO Roczniki Chemii (1961), 35, 979-84
CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA Unavailable
OS CASREACT 56:31702
AB Azlactones (I) of the formyl derivs. of the following amino acids were prepared by reaction of dicyclohexylcarbodiimide (II) with the corresponding acylamino acid in EtOAc: DL-alanine, m. 137-9° low yield; DL-valine, m. 177-8°, 55% yield; DL-norleucine, bl 47° 48.3% yield; L-leucine, b. 42-3°, 32.4% yield, [α]D -46.4°. I reacted easily with Et esters of amino acids to give the following: Et formyl-DL-valyl-DL-norleucinate (III) (m. 98-9°, quant. yield); Et formyl-L-leucylglycinate (m. 113-15° 72.5%, [α]D -7.1°); Et formyl-DL-norleucyl-L-leucinate (m. 120-2° 80%, -19.0°). III reacted similarly with II to give a tripeptide (m. 152°, 46%), and dicyclo-hexylurea (IV). The reaction of benzoyldiglycine with II led similarly to formation of IV but not to N-(benzoyldiglycyl)-N,N'-dicyclohexylurea (Khorana, CA 47, 1054g).
IT **93818-92-9**, Acetanilide, 2-(2-benzamidoacetamido)- (preparation of)
RN 93818-92-9 CAPLUS
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



L71 ANSWER 41 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1961:111878 CAPLUS
DN 55:111878
OREF 55:21015i,21016a-i,21017a-i,21018a-i,21019a-i,21020a-i,21021a-c
TI Chemotherapy of schistosomiasis. IV. Ethers of 4-amino-2-methoxyphenol
AU Collins, R. F.; Davis, M.
CS May & Baker, Ltd., Dagenham, UK
SO Journal of the Chemical Society, Abstracts (1961) 1863-79
CODEN: JCSAAZ; ISSN: 0590-9791
DT Journal
LA Unavailable
AB cf. CA 54; 7613f. Alkyl ethers of 4-amino-2-methoxyphenol (I) were prepared together with some related compds. and N-substituted derivs. Many of the compds. were schistosomicides. Benzylideneacetone was reduced catalytically in alc. to 92% 4-phenyl-2-butanol (II), b11 119-21°. II refluxed 20 hrs. with 50% HBr gave 75% 4-phenyl-2-butyl bromide (III), b10 116°. PhCH2MgCl (from 189.75 g. PhCH2Cl) in 400 cc. Et2O treated during 1 hr. with 2,3-dichlorotetrahydropyran (from 86 g. dihydropyran) in 200 ml. Et2O, the mixture stirred 5 hrs., left overnight, and decomposed gave 145.4 g. mixture containing both cis- and trans-2-benzyl-3-chlorotetrahydropyran (IV), b15 148-78°. Similar reactions were carried out with PhBr, PhCH2CH2Br, 3-phenylpropyl bromide, o-bromotoluene, p-bromotoluene, and p-bromoanisole. Crude IV (144 g.) added to 34.8 g. Na in 500 ml. Et2O and the mixture treated with 50 ml. alc. after standing overnight gave 107.7 g. trans-6-phenylhex-4-en-1-ol, b10 152-7°, n12D 1.5380. Similarly prepared (yields were for crude alc. over-all from dihydropyran) were trans-5-phenyl-4-penten-1-ol (77%), b0.1 102°, n20D 1.5620; trans-7-phenyl-4-hepten-1-ol (51%), b0.03 100-5°, nD 1.5260; trans-8-phenyl-4-octen-1-ol (81%), b15 190-4°, n19D 1.5240; trans-5-(o-tolyl)-4-penten-1-ol (49%), b15 162-70°, nD 1.5505; trans-5-(p-tolyl)-4-penten-1-ol (78%), b14 155-73°, m. 40-2°; trans-5-(p-methoxyphenyl)-4-penten-1-ol (71%), m. 74-5°. Catalytic reduction of the above unsatd. alcs. with Raney Ni gave resp.: 5-phenylpentanol (87%), b11 133-4°; 6-phenylhexanol (93%), b13 157-67°; 7-phenylheptanol (65%), b0.02 125-35°, nD 1.5135; 8-phenyloctanol (81%), b12 185-9°, n19D 1.5080; 5-(o-tolyl)pentanol (86%), b13 155-6°, nD 1.5225; 5-(p-tolyl)pentanol (95%), b14 159-62°; 5-(p-methoxyphenyl)pentanol (94%), b0.03 110-15°. The saturated alcs. were converted into the bromides by treatment with 50% aqueous HBr (2 ml./g.) and concentrated H2SO4 (0.67 ml./g.) 20 hrs. at 100°. The following were obtained: 5-phenylpentyl bromide; 6-phenylhexyl bromide; 7-phenylheptyl bromide, b0.05 110-14°; 8-phenyloctyl bromide (72%), b12 185-7°; 5-(o-tolyl)pentyl bromide (84%), b14 155-62°; 5-(p-tolyl)pentyl bromide (84%), b14 157-63°. 5-Phenyl-4-penten-1-yl p-toluenesulfonate (V), prepared in 38% yield in the usual way, m. 42-3° (MeOH). When V was prepared in C5H5N and the mixture left several days at room temperature the product was the quaternary pyridinium salt, m. 68-9°. 1-Methyl-5-phenylpentyl bromide prepared by catalytic reduction of cinnamylideneacetone and subsequent treatment with 50% HBr, b14 152-6°, n30D 1.5218. 5-Cyclohexylpentan-1-ol was prepared in 90% yield by reduction of 5-phenylpent-4-en-1-ol over Raney Ni in alc. at 131°/100 atmospheric, b11 136-7°, n17D 1.4685. Treatment with HBr-H2SO4 gave 91% 5-cyclohexylpentyl bromide, b7 127°, n20D 1.4838. NaNH2 (15.6 g.) powdered under 50 ml. PhMe for 30 hrs., treated under reflux with 19.65 g. 3-chlorotetrahydro-2-phenylpyran in 50 ml.

PhMe, and refluxed 17 hrs. gave 78% 3,4-dihydro-6-phenyl-2H-pyran, b9 119-25°, n17D 1.5703. When heated 15 min. at 100° with 50% HBr it gave 94% 4-benzoylbutyl bromide, m. 58°. 4-(p-Methoxyphenoxy)butyl bromide (67.5 g.) in 50 ml. alc. and 50 g. benzoylacetic ester added successively to 6.1 g. Na in 150 ml. alc., mixture refluxed 3 hrs., and concentrated gave 62 g. Et α-[4-(p-methoxyphenoxy)-butyl]benzoylacetate (VI), m. 38-40° (alc.). VI (50 g.), 20 g. KOH, 300 ml. MeOH, and 200 ml. H2O refluxed 24 hrs. gave 34.3 g. 1-benzoyl-5-(p-methoxyphenoxy)pentane (VII), m. 42°. The alkaline mother liquors on acidification gave 1 g. 6-(p-methoxyphenoxy)hexanoic acid, m. 80-2°. VII (34.5 g.), 30 g. PhOH, and 100 ml. 50% HBr refluxed 2 hrs., added to dilute NaOH, and extracted with Et2O gave 17.3 g. 5-benzoylpentyl bromide, b14 190-200°, m. 37.5-8.5° (ligroine). 1,5-Dibromopentane (46 g.) and 19.2 g. benzoylacetic ester added successively to 2.3 g. Na in 70 ml. alc., the mixture refluxed 1.5 hrs., and the residue treated with 100 ml. 50% HBr 18 hrs. on the steam bath gave 14.7 g. 6-benzoylhexyl bromide, b0.03 140-50°. K 2-methoxy-4-nitrophenoxide (220.5 g.), 1150 g. 1,5-dibromopentane, and 3 l. Me2CO refluxed 20 hrs., concentrated, steam distilled, and the residue extracted with CHCl3, concentrated, and diluted gave 252 g. crude bromide. This bromide was dissolved in Et2O and filtered from 8.85 g. 1,5-bis(2-methoxy-4-nitrophenoxy)pentane, m. 122-3°. Crystallization afforded 218 g. 3-(2-methoxy-4-nitrophenoxy)propyl bromide, m. 77.5-9.0° (MeOH). 7-(2-Methoxy-4-nitrophenoxy)-1-phenylheptan-1-ol (39 g.) treated at room temperature with 150 ml. Ac2O and 1 drop concentrated H2SO4 gave 37 g. 7-(2-methoxy-4-nitrophenoxy)-1-phenylheptyl acetate, m. 88-9° (MeOH). In another experiment the mixture was refluxed 1 hr. to give 7 g. 7-(2-methoxy-4-nitrophenoxy)-1-phenyl-1-heptene, m. 97-9°. Its structure was confirmed by catalytic reduction to 1-(4-amino-2-methoxyphenoxy)-7-phenylheptane. Similarly prepared was 71% 5-(2-methoxy-4-nitrophenoxy)-1-phenylpentyl acetate, m. 114-15°. 1-Benzoyl-4-(2-methoxy-4-nitrophenoxy)butane (15 g.) in 100 ml. alc. left 3 days at 35-40° with 5.8 g. HC(OEt)3 and 1 drop concentrated HCl gave 10.2 g. 5-(2-methoxy-4-nitrophenoxy)-1-phenylpentan-1-one diethyl acetal, m. 62-4° (Et2O-ligroine). Et α-[4-(p-nitrophenoxy)butyl]benzoylacetate (VIII), prepared in 62% yield from benzoylacetic ester and 4-(p-nitrophenoxy)butyl bromide, m. 74-5°. VIII (33.3 g.) hydrolyzed by refluxing 24 hrs. with 13 g. KOH in 250 ml. MeOH and 250 ml. H2O gave 80% 6-(p-nitrophenoxy)-1-phenylhexan-1-one (IX), m. 102° (alc.). 6-(p-Nitrophenoxy)hexanoic acid was isolated from the mother liquor in 1.8-g. yield, m. 103-4°. IX was obtained in 76% yield by condensation of K p-nitrophenoxide with 5-benzoylpentyl bromide. 5-(p-Nitrophenoxy)-1-phenylpentan-1-one was similarly obtained from benzoylacetic ester and 3-(p-nitrophenoxy)propyl bromide in 26% over-all yield. 5-(p-Nitrophenoxy)pentanoic acid was obtained in 13% yield from the alkaline liquors. The ketone had been synthesized by another route earlier. 6-(p-Nitrophenoxy)-1-phenylhexan-1-ol was prepared in 94% yield by reduction (Meerwein-Ponndorf method) of IX, m. 72-4°. 5-(2-Methoxy-4-nitrophenoxy)pentyl bromide (63.6 g.), 15.2 g. CS(NH2)2, and 150 ml. alc. refluxed 20 hrs. gave 93% S-[5-(2-methoxy-4-nitrophenoxy)pentyl]thiourea (X), m. 158-9° (alc.). X (95 g.) and 129 ml. 1.86N NaOH refluxed 3 hrs. and extracted with CHCl3 gave 79% 5-(2-methoxy-4-nitrophenoxy)pentane-1-thiol (XI), m. 84-6°. XI (6.15 g.) refluxed with 0.52 g. Na in 30 ml. alc. while 3.55 g. MeI in 10 ml. alc. was added during 15 min., after a further 4 hrs. the mixture evaporated, and the residue dissolved in CHCl3 gave 55% 1-(2-methoxy-4-

nitrophenoxy)-5-(methylthio)pentane, b0.15 185-205°, m. 56-9°. 2-Mercaptoethanol (15.6 g.) and 60.4 g. 5-(2-methoxy-4-nitrophenoxy)pentyl bromide added successively to 4.6 g. Na in 150 ml. alc. and the mixture refluxed 1 hr. gave 52% 1-(2-hydroxyethylthio)-5-(2-methoxy-4-nitrophenoxy)pentane, m. 52-4°. Similarly prepared were 80% 1-benzylthio-3-(2-methoxy-4-nitrophenoxy)propane, m. 51-3° (MeOH-alc.), 83% 1-(2-methoxy-4-nitrophenoxy)-5-(phenylthio)pentane, m. 54-5° (Et2O-ligroine), and 76% 1-(p-chlorophenylthio)-5-(2-methoxy-4-nitrophenoxy)pentane, m. 67-9° (alc.-Et2O). Similarly prepared, with 5-(p-nitrophenoxy)pentyl bromide, were 90% 1-(p-nitrophenoxy)-5-(phenylthio)pentane (XIa), m. 67° (alc.), 88% 1-(p-nitrophenoxy)-5-(p-nitrophenylthio)pentane, m. 83-4° (AcOH), and 77% 5-benzylthio-1-(p-nitrophenoxy)pentane, m. 33-4° (alc.). PhSH (11 g.) refluxed 0.5 hr. with 2.3 g. Na in 100 ml. alc. and 1,3-dibromopropane gave 3-phenylthiopropyl bromide and this was condensed with K 2-methoxy-4-nitrophenoxide to give 54% 1-(2-methoxy-4-nitrophenoxy)-3-(phenylthio) propane (XII), m. 87-9° (alc.). XII (27 g.) in 200 ml. AcOH treated with 20 ml. 30% H2O2 (the temperature rose to 50°), after 2.5 hrs. the solution heated 1 hr. at 90°, and poured into H2O gave 88% 1-(2-methoxy-4-nitrophenoxy)-5-(phenylsulfonyl) pentane, m. 122-4° (alc.). Similarly prepared were: 66% 1-(2-methoxy-4-nitrophenoxy)-5-(methylsulfonyl)pentane, m. 95-7°; 97% 1-(p-nitrophenoxy)-5-(phenylsulfonyl)pentane, m. 85-6° (alc.); 94% 1-(p-nitrophenoxy)-5-(p-nitrophenylsulfonyl)pentane, m. 129-30° (AcOH); 88% 1-benzylsulfonyl-5-(p-nitrophenoxy)pentane, m. 120-1° (AcOH). 5-(p-Nitrophenoxy)pentyl bromide (28.8 g.), 19.9 g. p-acetamidobenzenesulfinic acid, 7 g. NaOAc, 2 g. NaI, 200 ml. 2-ethoxyethanol, and 5 ml. H2O refluxed 2.5 hrs., concentrated, and diluted with Et2O gave 55% 1-(p-acetamidophenylsulfonyl)-5-(p-nitrophenoxy)pentane, m. 112-13° (alc.). XIa (40 g.) in 400 ml. AcOH treated at 40° with 14.6 ml. 30% H2O2 and the solution heated 0.5 hr. at 80° gave 98% 5-(p-nitrophenoxy)pentyl phenyl sulfoxide, m. 80-1° (alc.). Similarly prepared was 92% benzyl 5-(p-nitrophenoxy)pentyl sulfoxide, m. 97-8° (aqueous alc.). K 2-methoxy-4-nitrophenoxide (14.1 g.), 28 g. acetobromoglucose, and 100 ml. HCONMe2 stirred 20 hrs. and the product in C6H6 stirred with activated Al2O3 gave 49% 2-methoxy-4-nitrophenyl tetra-O-acetyl-D-glucoside (XIII), m. 145-7°. XIII was obtained in traces by using the free phenol, Ag2CO3, quinoline, and acetobromoglucose in Et2O. XIII (33.2 g.) in 340 ml. MeOH kept 0.5 hr. in a solution of 11.2 g. NaOH, H2O, and 170 ml. MeOH gave 2-methoxy-4-nitrophenyl D-glucoside, m. 212-13°. 2-Methoxy-4-nitrophenol (31 g.) reduced over PtO2 in alc. and the residue acetylated gave 50% 4-acetamido-2-methoxyphenyl acetate (XIV), m. 150-2°. XIV (54 g.) shaken 10 min. with 242 ml. 2N NaOH containing wetting agent gave 98% 4-acetamido-2-methoxyphenol (XV), m. 115-17° (EtOAc). XV (15.35 g.) and 23.1 g. 5-(p-nitrophenyl)pentyl bromide refluxed 20 hrs. with 1.95 g. Na in 100 ml. alc. gave 21% 1-(4-acetamido-2-methoxyphenoxy)-5-(p-nitrophenyl)pentane, m. 115.5-16.0° (MeOH). 4-Nitropyrocatechol (18.2 g.) and 34.7 g. 5-phthalimidopentyl bromide refluxed 20 hrs. with 100 ml. EtOCH2CH2OH and 6.6 g. KOH in 20 ml. H2O gave 41% 1-(2-hydroxy-4-nitrophenoxy)-5-phthalimidopentane (VXI), m. 137-9° (AcOH). XVI (0.77 g.), 0.3 g. anhydrous K2CO3, 4 ml. MeI, and 30 ml. Me2CO refluxed 20 hrs. gave 1-(2-methoxy-4-nitrophenoxy)-5-phthalimidopentane, m. 147.5-8.5° (aqueous alc.). 1-(2-Methoxy-5-nitrophenoxy)-5-phenylpentane, m. 73-5° (alc.), was prepared in 81% yield from 2-methoxy-5-nitrophenol, 5-phenylpentyl bromide, and 10N KOH in EtOCH2CH2OH. HNO3 (20 ml.) added

slowly to 30 g. 1,2,3-trimethoxybenzene in 60 ml. AcOH, cooled when the temperature reached 90-100°, and the product stirred with hot dilute NaOH gave 39-41% 1,2,3-trimethoxy-5-nitrobenzene (XVII). XVII (60 g.) refluxed 2 days with 60 g. KOH in 350 ml. H2O, the 49.5 g. K salt filtered off, washed, dried, and the mother liquors afforded 6.1 g. more salt. 1,3-Dimethoxyacetone (7.14 g.), 9.5 g. Na nitromalonaldehyde, and 0.9 g. NaOH in 90 ml. H2O kept overnight at room temperature gave 8.35 g. Na salt. Acidification gave 2,6-dimethoxy-4-nitrophenol, m. 136-7° (effervescence). The above K salt (40 g.), 50 g. 5-phthalimidopentyl bromide, and 100 ml. EtOCH2CH2OH refluxed 7 days at 100° gave 68% 1-(2,6-dimethoxy-4-nitrophenoxy)-5-phthalimidopentane, m. 105-6°. Similarly obtained (63%) (refluxed for 48 hrs.) was 1-(2,6-dimethoxy-4-nitrophenoxy)-5-phenylpentane, m. 36-7° (ligroine). Nitro compds., 2,4-MeO(O2N)C6H3O(CH2)nR, were prepared (except where stated) by condensation of 2,4-MeO(O2N)C6H3OK with the appropriate alkyl bromide, usually in refluxing alc. or EtOCH2CH2OH. The following compds. were obtained (n, R, % yield, m.p., and solvent given): 4, Me, 71, 54-5°, alc.; 5, Me, 69, 69.5-70.5°, alc.; 6, Me, 63, 53-5°, alc.; 7, Me, 87, 37-8°, alc.-H2O; 8, Me, -, -, -; 9, Me, 73, 50°, alc.; 10, Me, 87, 49.5-50.5°, alc.; 11, Me, 73, 51-2.5°, alc.; 15, Me, 73, 57-8.5°, alc.; 1, CHEt2, 45, - (b0.05 150-70°), -; 1, CHEtBu, 44, - (b0.02 164-8°), -; 0, CHMeC6H13, 18, 42-3°, MeOH; 1, CHMeCH2CMe3, -, noncryst., -; 0, CHMeC7H15, 19 (p-toluenesulfonate of the alc. used), - (b0.8 186-94°), -; 2, CHMe(CH2)2CH2Pr-iso, 29, -(b0.3 204-15°), -; 0, cyclopentyl, 53, 83-5°, alc.; 2, cyclohexyl, 64, 78-80°, alc.; 5, cyclohexyl, 66, 57-8°, ligroine; 1, CH:CH2, 85, 51-2.5°, Et2O-ligroine; 3, CH:CH2, 68, 65-6°, alc.-H2O; 2, CH:CHBu, 36 (over-all from 3-hepten-1-ol via the p-tosylate), - (b0.1 164-86°), -; 1, COMe, 63, 116-18°, alc.; 5, OAc, 89 (from nitroguaiacyloxypentyl bromide and KOAc), 75-6°, alc.; 1, CO2Et, 79 (via p-tosylate), 86-8°, MeOH; 1, CO2H, 91 (by hydrolysis of the Et ester with 0.8N NaOH), 165.5-7.0°, AcOH-H2O; 2, NEt2, 49 (from CH2ClCH2NEt2 in Me2CO), - (b0.15 175-200°), - 1, Ph, 70, 80-2°, HO(CH2)2OEt; 2, Ph, 66, 97-9°, alc.; 3, Ph, 85, 72.5-3.5°, alc.; 4, Ph, -, -, -; 0, CHMe(CH2)2Ph, 55, 50-1°, alc.; 5, Ph, 81 (over-all from 5-phenylpentanol), 75-6, alc.; 6, Ph, -, 55-7°, ligroine; 0, CHMe(CH2)4Ph, 58, 65.5-7.5°, Et2O-ligroine; 7, Ph, 59, 73-4°, alc.; 8, Ph, 62, 49-50°, Me2CO-alc.; 5, C6H4Meo, 84, 76-8°, alc.; 5, C6H4OMe-p, 57 (over-all from 5-(p-methoxyphenyl)pentanol), 81-2°, alc.; 5, C6H4NO2-p, 45, 84 and 93-4°, Me2CO-alc.; 5, C6H3(NO2)2-2,4, 58, 86-7°, EtOAc; 3, CH:CHPh-trans, 74, 95-7°, alc.; 3, CH:CHC6H4Me-p-trans, 57, 103-3.5°, EtOAc-ligroine; 3, CH:CHC6H4OMe-p-trans, 60 (over-all from 5(p-methoxyphenyl)-4-penten-1-ol), 121-1.5°, alc.-EtOAc; 1, p-C6H4SO2Me, 87, 195-7°, alc.; 1, 1-naphthyl, 62, 110-11°, alc.-Me2CO; 1, OMe, 82 (from CH2ClOMe), 89-92°, alc.-ligroine; 5, OMe, 66, (b0.1 170°), -; 2, OCH2Ph, 80 (p-tosylate), 75-7°, alc.; 5, OCH2Ph, 71 (from 5-benzyloxypentyl bromide), 90-1°, alc.; 2, OPh, 90, 116-17°, alc.; 3, OPh, 73, 100-2°, alc.; 4, OPh, 89, 90-1.5°, alc.; 5, OPh, 80, 67-8°, alc.; 6, OPh, 84, 81-2°, alc.; 7, OPh, 70, 56-7°, alc.; 8, OPh, 82, 58-9°, alc.; 3, OC6H4OMe-p, 32, 96-7°, alc.; 4, OC6H4OMe-p, 85, 106-7°, alc.; 5, OC6H4NHAc-p, 78, 95-6°, AcOH; 5, phthalimido, 78 (noncryst.), 147.5-8.5°, AcOH; 6, phthalimido, 61, 81-3°, alc.; 8, phthalimido, 79, 91-2°, AcOH; 5, NHCOPh, 64, 131-2°, EtOAc; 5, NHCOCH2NHCOPh, 95, 129-30° (b0.02 164-84°), Me2CO; 5, NHCO(CH2)3CO2H, 99, 94-7°,

Me2CO-ligroine; 5, glutarimido, 83, 138-40°, alc.; 1, COPh, 84, 122-3°, EtOCH2CH2OH; 4, COPh, 59, 91°, EtOCH2CH2OH; 6, COPh, 81, 82-4°, alc.; 4, CHPhOH, 94, 76-7°, Et2O-ligroine; 6, CHPhOH, 89, 62-3°, Et2O-ligroine. 5-(2-Methoxy-4-nitrophenoxy)pentyl bromide (24 g.), 48 g. Na2S.9H2O, 200 ml. alc., and 100 ml. H2O refluxed 24 hrs., and the product purified via the HCl salt, and liberated gave bis[5-(4-amino-2-methoxyphenoxy)pentyl] sulfide, m. 90-2° (CHCl3-Et2O). 3,3' - Dimethoxy - (4,4' - bisoctyloxy)azoxybenzene was prepared in 5% yield, m. 86-9°, when a batch of 1-(2-methoxy-4-nitrophenoxy)octane was reduced over Raney Ni in alc. The principal product, 3-methoxy-4-(octyloxy)aniline, was isolated from the filtrate. The corresponding nitro compound (15.6 g.) in 460 ml. alc. and 180 ml. H2O reduced over Raney Ni gave 70% 4-amino-2-methoxyphenyl D-glucoside, m. 202-3°, [α]19.5D -61° (H2O). 3,5-Dimethoxy-4,5'-phthalimidopentylaniline was obtained in 85% yield by catalytic reduction of the nitro compound over Raney Ni, m. 97°. 3,5-Dimethoxy- m. 85-7° (Et2O), and 3-methoxy-4-(5-phenylpentyloxy)aniline (92%), m. 59-60° (Et2O-ligroine) [methanesulfonate m. 130-1° (alc.-Et2O)], were obtained by a similar reduction in alc. The following 2,4-MeO(H2N)C6H3O(CH2)nR were prepared by catalytic reduction of the corresponding nitro compds., usually over Raney Ni in alc. or EtOCH2CH2OH, but occasionally in EtOAc or HCONMe2 (n, R, base or derivative, % yield, m.p., solvent given): 1, Me, base, 86, 60-1°, Et2O-ligroine; 2, Me, base, 87, 65-7°, Et2O-ligroine; 3, Me, base, 77, 35-6°, ligroine; 3, Me, MeSO3H salt, -, 173-5°, alc.; 4, Me, base, 92, 43-4°, ligroine; 4, Me, HCl salt, -, 185-200°, alc.-Et2O; 5, Me, base, 91, 67-9°, alc.; 5, Me, HCl salt, -, 185-200°, alc.-Et2O; 6, Me, base, 92, 72-4°, alc.; 7, Me, base, 76, 63-4°, EtOH, 7, Me, MeSO3H salt, -, 120-5° and 200°, -; 7, Me, di-p-toluoyl-D-tartrate -, 161-2°, EtOAc; 8, Me, base, 64 (over-all from K nitrogauiacyl oxide), 71-3°, Et2O-ligroine; 9, Me, base, 84, 61-2°, ligroine; 10, Me, base, 95, 66-7°, alc.; 11, Me, base, 90, 65-6°, alc.; 15, Me, base, 85, 67-8°, Et2O-ligroine; 1, CHEt2, HBr salt, 69, 214-17°, alc.-Et2O; 1, CHEtBu, HBr salt, 55, 160-4°, Et2O-C6H6;

0, CHMeC6H13, base, 83, b0.05 143-6°, -; 2, CHMeCH2CMe3, base, 62 (di-p-toluoyl-D-tartrate), 72-3.5°, Et2O-ligroine; 0, CHMeC6H13, HCl, -, 160-80°, alc.-Et2O; 0, CHMeC7H15, base, 49, b0.2 160-70°, -; 0, CHMeC7H15, HCl salt, -, 164-8°, -; 2, CHMe(CH2)2CH2Pr-iso, HCl salt, 59, 158-64°, alc.-Et2O; 0, cyclopentyl, base, 83, 64-6°, alc.-ligroine; 2, cyclohexyl, base, 80, 64-5°, ligroine; 5, cyclohexyl, base, 80, 91-1.5°, MeOH; 3, CH:CH2, base, 90 (from the corresponding nitro ketone), 25-6°, Et2O-ligroine; 3, CH:CH2, HBr salt, -, 195-7°, dilute aqueous HBr; 2, CH:CHBu, base, 42 (from the corresponding nitro ketone), 38-42°, ligroine; 1, CHMeOH, base, 78 (from the corresponding nitro ketone), 125-6°, alc.; 5, OAc, base, 71, 46-8°, alc.-H2O; 5, OH, base, 93 (by acid hydrolysis of the acetate), 70-1°, CHCl3-ligroine; 1, CO2H, base, 93, 200-2°, H2O; 2, NEt2, di-HBr salt, 81, 216-18°, MeOH-Et2O; 1, Ph, base, 39, 84-5°, ligroine (b. 100-20°); 1, Ph, MeSO3H salt, -, 200-1°, alc.-Et2O; 2, Ph, base, 78, 47-8°, Et2O-ligroine; 2, Ph, MeSO3H, -, 159-60°, alc.-Et2O; 3, Ph, base, 90, 103-4°, alc.; 3, Ph, MeSO3H salt, -, 159-60°, alc.-Et2O; 4, Ph, MeSO3H, 60, 123-4°, alc.; 5, Ph, base, 90 [from 1-(2-methoxy-4-nitrophenoxy)-5-nitropentane], 77-8°, alc.; 5, Ph, MeSO3H salt, 86 [from 1-(2-methoxy-4-nitrophenoxy)-5-phenyl-4-pentene], 138.5-9.5°, -; 5,

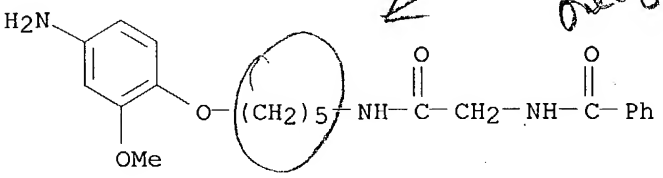
Ph, HCl salt, -, 147-9° (clears 158-60°), alc.-Et2O; 6, Ph, base, 38 (over-all from 6-phenylhexanol), 39-41°, Et2O-ligroine; 0, CHMe(CH2)4Ph, base, 70, 42-4°, Et2O-ligroine; 7, Ph, base, 80, 65°, alc.-ligroine; 8, Ph, base, 87, 52-3°, Et2O-ligroine; 5, C6H4Me-o, base, 73, 69-71°, alc.-H2O; 5, C6H4Me-p, base, 91, 84-6°, alc.-ligroine; 5, C6H4OMe-p, base, 93, 98-100°, alc.; 5, C6H4NO2-p, base, 82 (from the N-acyl derivative by hydrolysis with 2N HCl in alc.), 86-7°, alc.; 5, C6H4NH2-p, base, 90, 68-9°, Et2O; 5, C6H3(NH2)2-2,4, base, 71, 99-100°, alc.-ligroine; 3, CH:CHPh-trans, base, 94 (reduction by Na2S in alc.), 90-2°, alc.-Et2O; 3, CH:CHPh-trans, MeSO3H, -, 188-90°, alc.-Et2O; 3, CH:CHC6H4Me-p-trans, base, 88 (reduction by Na2S in alc.), 117-18°, alc.; 1, 1-naphthyl, base, 65, 61-3°, Et2O; 1, 1-naphthyl, MeSO3H salt, -, 192-4°, alc.; 1, C6H4SO2Me-p, base, 85, 130°, HO(CH2)2OEt-Et2O; 1, OMe, base, 80, 61-2°, alc.-Et2O; 5, OMe, base, 78, -(b0.1 160-5°), -; 5, OMe, MeSO3H salt, 88, 124-6°, alc.-Et2O; 2, OCH2Ph, base, 88, 41-2°, alc.-ligroine; 2, OCH2Ph, MeSO3H salt, -, 138-9°, alc.-Et2O; 5, OCH2Ph, base, 80, 34-5°, ligroine; 5, OCH2Ph, MeSO3H salt, -, 122-4°, alc.-Et2O; 2, OPh, base, 84, 106-7°, alc.; 3, OPh, base, 81, 76-8°, alc.; 4, OPh, base, 74, 115-17°, alc.; 5, OPh, base, 81, 76-8°, alc.; 5, OPh, MeSO3H salt, 83, 125°, alc.-Et2O; 6, OPh, base, 75, 104-4.5°, alc.; 7, OPh, base, 73, 57-8°, alc.; 8, OPh, base, 78, 76-7°, CCl4; 3, OC6H4OMe-p, base, 79, 66-7.5°, alc.; 4, OC6H4OMe-p, base, 74, 105-7°, alc.; 5, OC6H4NHAc-p, MeSO3H salt, 74, 167-9°, alc.; 5, OC6H4NH2-p, di-MeSO3H salt, 64, 232-4°, alc.; 5, phthalimido, base, 61, 103-5°, alc.; 5, phthalimido, MeSO3H, 92, 205-7°, alc.-Et2O; 6, phthalimido, base, 98, 86-7°, alc.; 8, phthalimido, base, 82, 70-1°, alc.; 5, NHCOPh, base, 82, 103-4°, C6H6; 5, NHCOCH2NHBz, base, 61, 120.5-1.5°, C6H6; 5, glutarimido, base, 83, 94-5°, alc.; 5, phthalimidino, base, 76 (from a phthalimide by reduction with Sn and HCl), 129-30°, alc.; 1, CHPhOH, base, 51 (from corresponding nitro ketone), 96-7°, alc.-H2O; 4, CHPhOH, base, 73° (from the corresponding nitro ketone), 104-5°, alc.; 6, CHPhOH, base, 89 (from the corresponding nitro ketone), 108-10°, alc.; 4, CHPhOAc, base, 72, 67-8°, Et2O; 6, CHPhOAc, base, 74, 36-7°, Et2O-ligroine; 4, COPh, base, 61 (reduction of the NO2 group by Fe and AcOH), 101-3°, MeOH; 6, COPh, base, 83 (reduction of NO2 by Fe and AcOH), 85-7°, EtOAc-Et2O; 4, CHPh(OEt)2 (sic), base, 78, 107-9°, MeOH; 5, SMe, base, 58 (reduction by Na2S in alc.), 53.5-6.0°, alc.-H2O; 5, S(CH2)2OH, base, 41 (Na2S in alc.), 38-40°, Et2O; 3, SCH2Ph, MeSO3H salt, 62 (Na2S in alc.), 134-6°, MeOH; 3, SPh, base, 75 (Na2S in alc.), 57-8°, alc.-Et2O; 5, SPh, base, 74 (Na2S in alc.), 72-3°, alc.-Et2O; 5, SC6H4Cl-p, base, 81 (Na2S in alc.), 44-6°, Et2O-ligroine; 5, SO2Me, base, 87, 84-7°, MeOH; 5, SO2Ph, base, 73, 89-90°, alc. The following p-H2NC6H4O(CH2)nR were similarly obtained (n, R, derivative, % yield, m.p., and solvent given): 4, COPh, base, 49° (nitro ketone reduced with Fe in 90% AcOH), 112-14°; 5, COPh, base, 56 (nitro ketone reduced with Fe in 90% AcOH), 61-3°, C6H6-ligroine; 5, CHPhOH, base, 89 (catalytic reduction of either nitro ketone or nitro alc.), 86-8°, Et2O-ligroine; 5, SPh, base, 92 (Na2S in alc.), 63, C6H6-ligroine; 5, SC6H4NH2-p, 2HCl, 66 (Na2S in alc.), 220-30° (decomposition), dilute HCl; 5, SCH2Ph, MeSO3H salt, 91 (Na2S in alc.), 147-9°, alc.-Et2O; 5, SOPh, base, 65 (Na2S in alc.), 70-1°, Et2O; 5, SOCH2Ph, base, 66 (Na2S in alc.), 89-90°, Et2O; 5, SO2Ph, base, 82, 93-5°, alc.; 5, SO2C6H4NH2-p, base, 84, 136-8°,

alc.; 5, SO2C6H4NH2-p, diacetyl, -, 154°, -; 5, SO2C6H4NHAc-p, base, 87, 126-8°, alc.; 5, SO2CH2Ph, base, 94, 101-2°, alc. N-Formyl-3-methoxy-4-(5-phenylpentyloxy)aniline, prepared in 89% yield from the primary amine by means of HCONH2 and concentrated HCl, m. 86-8° (MeOH). The 4-octyloxy derivative (81%), m. 77-8° (MeOH), was similarly prepared The following formamides were reduced with LiAlH4 in Et2O-C6H6. The resulting primary amines were converted into the quaternary iodides, which were pyrolyzed in vacuo. 2-Chloroethyl chloroformate (8.7 g.) and 11.1 g. NaOAc.3H2O added successively to 20 g. 3-methoxy-4-(5-phenylpentyloxy)aniline suspended in 115 ml. H2O and 3 ml. AcOH, the mixture shaken 1 hr., and the solid washed gave 85% N-(2-chloroethoxycarbonyl)-3-methoxy-4-(5-phenylpentyloxy)aniline (XVIII), m. 76-8.5° (aqueous alc.). XVIII (22.4 g.) added to 12 g. NaOH in 23 ml. H2O, 4.9 ml. alc., and 49 ml. EtOCH2CH2OH, and the mixture refluxed 10 min. gave 68% N-(2-hydroxyethyl)-3-methoxy-4-(5-phenylpentyloxy)aniline, m. 72-3° (aqueous alc.). 3-Methoxy-4-(5-phenylpentyloxy)aniline (14.27 g.), 14.27 g. CaCO3, 14.27 ml. CH2ClCH2OH, and 150 ml. H2O refluxed 18 hrs., extracted with CHCl3, and the residue treated with MeSO3H in alc.-Et2O gave 46% N,N-bis(2-hydroxyethyl)-3-methoxy-4-(5-phenylpentyloxy)aniline, m. 93-4°. 3-Methoxy-4-(5-phthalimidopentyloxy)aniline (20 g.), 25 ml. 1,2-epoxypropane, 170 ml. alc., and 1 ml. concentrated HCl refluxed 24 hrs. gave 28% N,N-bis(2-hydroxypropyl)-3-methoxy-4-(5-phthalimidopentyloxy)aniline, m. 112-14° (MeOH-Et2O). 3-Methoxy-4-(5-phthalimidopentyloxy)aniline (3.54 g.), 1.8 g. D-glucose, and 30 ml. alc. refluxed 1.5 hrs. gave 53% N-(D-glucosyl)-3-methoxy-4-(5-phthalimidopentyloxy)aniline, m. 121-3°. Similarly prepared was 62% of the corresponding galactosylamine, m. 96-8°.
3-Methoxy-4-octyloxyaniline (30 g.), 10 g. dicyandiamide, 10 ml. concentrated HCl, and 300 ml. Me2CO refluxed 4 hrs. gave 4,6-diamino-1,2-dihydro-1-(3-methoxy-4-octyloxyphenyl)-2,2-dimethyl-1,3,5-triazine HCl salt, m. 210-12°. The following 2,4-MeO(R1R2N)C6H3O(CH2)nR were prepared (R1, R2, n, R, base or derivative, % yield, m.p., and solvent given): Me, H, 5, Ph, base, 63, 35° (b0.04 197-228°), Et2O-ligroine; Me, H, 7, Me, base, 63, b0.2 161-3°, -; Me, Me, 2, Ph, base, 93, 32-3°, Et2O; Me, Me, 2, Ph, MeI salt, 89, 152-6°, H2O; Me, Me, 5, Ph, base, 93, 38.5-9.5°, Et2O-ligroine; Me, Me, 5, Ph, MeI salt, 93°, 183-5°, H2O; Me, Me, 5, Ph, p-C6H4MeSO3H salt, -, 114-16°, alc.-Et2O; Me, Me, 7, Me, HBr salt, 80, 119-20°, alc.-Et2O; Me, Me, 7, Me, MeI salt, 67, 184-6° (decomposition), H2O; Me, Me, 4, OPh, base, 89, 49-51°, Et2O-ligroine; Me, Me, 4, OPh, MeI, 95, 162.5-4.0° (decomposition), H2O; Me, Me, 4, COPh, base, 73, 82-4°, alc.; Me, Me, 4, COPh, MeI salt, 92, 160-3° (decomposition), H2O; Me, Me, 5, SPh, HBr, 26, 96-8°, aqueous HBr; Me, Me, 5, SPh, MeI, 100, 142-5° (decomposition), H2O; Me, Me, 5, p-C6H4NMe2, base, 74, 39-41°, ligroine; Me, Me, 5, p-C6H4NMe2, MeI salt, 80, 203-4°, H2O; Me, Me, 5, phthalimido, base, 92, 70-2°, alc.; Et, Et, 7, Me, base, 85° (over-all from primary amine), -, -; Me, Me, 5, phthalimido, MeI salt, 100, 200-2°, H2O; CO2CH2CH2Cl, H, 2, Ph, -, 90, 63-5°, alc.; CO2CH2CH2Cl, H, 7, Me, -, 100, 72-3.5°, alc.; CO2CH2CH2Cl, H, 4, OPh, -, 94, 109-10°, alc.; CO2CH2CH2Cl, H, 4, COPh, -, 69, 95-7°, alc.; CO2CH2CH2Cl, H, 5, SPh, -, 86, 45-7°, alc.-H2O; (CH2)2OH, H, 2, Ph, HBr, 75, 147.5-9.0°, MeOH-Et2O; (CH2)2OH, H, 7, Me, base, 75, 35-6°, ligroine; (CH2)2OH, H, 4, OPh, base, 87, 62.5-3.5°, MeOH; (CH2)2OH, H, 4, COPh, base, 86, 77-8°, alc.-Et2O; (CH2)2OH, H, 5, SPh, HBr, 67, 113-15°, alc.-Et2O; (CH2)2OH, (CH2)2OH, 7, Me, base, 34, 62-4°, Et2O; (CH2)2OH, (CH2)2OH, 5, phthalimido, base, 51, 68-9°, alc.

IT **103506-85-0**, Benzamide, N-{{[5-(4-amino-2-methoxyphenoxy)pentyl]carbamoyl}methyl}- **103990-63-2**, Benzamide, N-{{[5-(2-methoxy-4-nitrophenoxy)pentyl]carbamoyl}methyl}-
(preparation of)

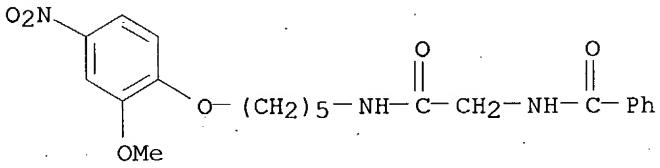
RN 103506-85-0 CAPLUS

CN Benzamide, N-[[[5-(4-amino-2-methoxyphenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)

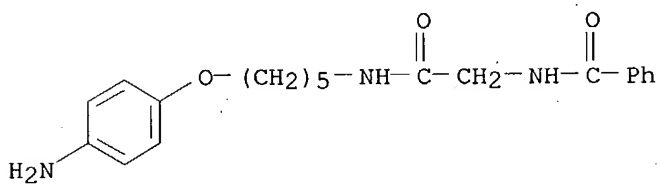


RN 103990-63-2 CAPLUS

CN Benzamide, N-[[[5-(2-methoxy-4-nitrophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



L71 ANSWER 42 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1960:87613 CAPLUS
DN 54:87613
OREF 54:16655a-d
TI The schistosomicidal and toxic effects of some N-(p-aminophenoxyalkyl)amides
AU Collins, R. F.; Davis, M.; Edge, N. D.; Hill, J.; Reading, H. W.; Turnbull, Eleanor R.
CS May & Baker Ltd., Dagenham, UK
SO British Journal of Pharmacology and Chemotherapy (1959), 14, 467-75
CODEN: BJPCAL; ISSN: 0366-0826
DT Journal
LA Unavailable
AB Compds. related to N-(p aminophenoxyalkyl)amide were prepared, and 102 were screened for schistosomicidal activity. Two of these compds., N-[5-(p-aminophenoxy)pentyl]phthalimide (I) and N-[5-(p-aminophenoxy)pentyl]benzamide (II) were investigated in detail. Given orally, I was inactive against Schistosoma mansoni in monkeys, but both I and II were effective in mice and hamsters. II was more toxic in rats, guinea pigs, and monkeys than I. Visual impairment in monkeys and cats by both compds. was considered to be less than other ω-p-aminophenoxyalkyl derivs. not containing an amide group. Results of absorption studies of the 2 compds. in rats and mice show lower blood concentration after 4 hrs. Most of the drug was excreted in the 1st 24 hrs. I has been found to be moderately effective against S. haematobium infections in Africans.
IT **103388-58-5**, Benzamide, N-{{[5-(p-aminophenoxy)pentyl]carbamoyl}methyl}-
(pharmacology of)
RN 103388-58-5 CAPLUS
CN Benzamide, N-[[[5-(p-aminophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



L71 ANSWER 43 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1960:38924 CAPLUS
DN 54:38924
OREF 54:7613f-i,7614a-i,7615a-i,7616a-i,7617a-i,7618a-d
TI Chemotherapy of schistosomiasis. III. N-(p-amino-phenoxyalkyl)amides, -imides, and -sulfonamides
AU Ashley, J. N.; Collins, R. F.; Davis, M.; Sirett, N. E.
CS May & Baker, Dagenham, UK
SO Journal of the Chemical Society, Abstracts (1959) 3880-94
CODEN: JCSAAZ; ISSN: 0590-9791
DT Journal
LA Unavailable
AB cf. C.A. 53, 17942c. Many acyl- and diacylaminoalkyl ethers of p-aminophenol (I) were prepared by a number of routes. Some of these compds. were effective against schistosomicides. K p-nitrophenoxide and 2-phthalimidoethyl bromide gave 22% 1-(p-nitrophenoxy)-2-phthalimidoethane, m. 152-4° (AcOH). Similarly prepared in either alc. or EtOCH2-CH2OH were: 44% 1-(p-nitrophenoxy)-3-phthalimidopropane, m. 189-91.5° (dioxane); 64% 1-(p-nitrophenoxy)-4-phthalimidobutane, m. 119° (AcOH); 60% 1-(p-nitrophenoxy)-10-phthalimidodecane, m. 102-3° (AcOH); and 55% 1-(p-nitrophenoxy)-6-phthalimido-3-hexene [from 6-phthalimido-1-(p-toluenesulfonyloxy)-3-hexene], m. 118-19° (aqueous AcOH). 1-(p-Nitrophenoxy)-5-phthalimidopentane (Ia) treated with aqueous N2H4.H2O in alc. and the amine liberated by shaking the complex with CHCl3 and warm 2N NaOH gave 1-amino-5-(p-nitrophenoxy)pentane (II), b0.02 160-5°. Similarly prepared were: 94% 1-amino-5-(p-aminophenoxy)pentane, m. 67-9° (ligroine) (dimethanesulfonate m. 244-6°); and 91% 1-(p-acetamidophenoxy)-5-aminopentane (IIa) m. 137-9° (C6H6) (methanesulfonate m. 155-7°). II (22.4 g.) and 28.6 g. tetrachlorophthalic anhydride heated 2 hrs. at 180-90°, cooled, and dissolved in 150 ml. hot EtOCH2CH2OH gave 96 % 1-(p-nitrophenoxy)-5-tetrachlorophthalimidopentane, m. 165-7°. Similarly prepared were: 84% 1-(p-nitrophenoxy)-5-(3-nitrophthalimido)pentane, m. 163-4.5°; 67% 1-(p-acetamidophenoxy)-5-(3-nitrophthalimido)pentane, m. 132-4°(alc.); and 65% 1-homophthalimido-5-(p-nitrophenoxy)pentane, m. 144-5° (Me2CO). 1-(p-Nitrophenoxy)-5-ureidopentane (61 g.), 24 g. CH2(CO2H)2, and 55 ml. AcOH heated to 70-80°, treated dropwise with 45 ml. Ac2O, left 8 hrs. at 90°, cooled, diluted with 84 ml. H2O, and filtered gave a solid, m. 178.5-80.0°, possibly an Ac derivative Further dilution with 240 ml. H2O gave 1-[5-(p-nitrophenoxy)pentyl]barbituric acid, m. 149-51° (alc.). II (45 g.) and 15.2 g. Me salicylate heated 5 hrs. at 120°, dissolved in CHCl3, washed with 2N HCl, dried, and evaporated gave 73% 1-(p-nitrophenoxy)-5-(salicylylamido)pentane (III), m. 123-5°(C6H6). ClCO2Et (12 g.) slowly added to a cold solution of 35 g. III in 120 ml. C6H6, the mixture heated 2 hrs. at 100°, cooled, and diluted with H2O gave 86% 3,4-dihydro-3-[5-(p-nitrophenoxy)pentyl]-2,4-dioxo-5,6-benz-1,2-oxazine, m. 145-6° (AcOH and alc.). 5-(p-Nitrophenoxy)pentyl bromide (IIIa) (16.15 g.), 10.15 g. (±)-camphorimide, 5.4 ml. 10.4N KOH, and 25 ml. EtOCH2CH2OH refluxed 2 hrs. and the product crystallized gave 71% 1-camphorimido-5-(p-nitrophenoxy)pentane, m. 66-7° (aqueous alc.). N-[5-(p-Nitrophenoxy)pentyl]phthalhydrazide was similarly obtained in 23% yield, m. 160-2° (PhMe). II (22.4 g.) in 100 ml. CHCl3 refluxed 1 hr. with 9.8 g. maleic anhydride in 100 ml. CHCl3 gave 53% 1-(β-carboxyacrylamido)-6-(p-nitrophenoxy)pentane (IV), m. 91-3° (alc.). Similarly prepared were: 63% 1-(p-acetamidophenoxy)-5-

(β-carboxyacrylamido)pentane, m. 161-3° (aqueous AcOH); 1-(β-carboxymethyl-β-methylvaleramido)-5-(p-nitrophenoxy)pentane (not obtained crystalline); and 92% 1-(γ-carboxybutyramido)-5-(p-nitrophenoxy)pentane (V), m. 116-17°. IV (17.2 g.), 18 ml. Ac2O, and 1.8 g. freshly fused NaOAc stirred 1 hr. at 100° gave 51% 1-maleimido-5-(p-nitrophenoxy)pentane, m. 105-7° (ligroine). The glutaramic acid (37.3 g.) and 100 ml. AcCl refluxed 20 min., evaporated, and the residue crystallized gave 84% 1-glutarimido-5-(p-nitrophenoxy)pentane, m. 87-8°(MeOH). 1-(β-Ethyl-β-methylglutarimido)-5-(p-nitrophenoxy)pentane was made similarly, but was not obtained crystalline Glutarimide (11.3 g.) and 28.8 g. 5-(p-nitrophenoxy)pentyl bromide refluxed 20 hrs. with 2.3 g. Na in 150 ml. alc., diluted with H2O, and extracted with CHCl3 gave 39% 1-(γ-ethoxycarbonylbutyramido)-5-(p-nitrophenoxy)pentane (VI), m. 90-1.5° (C6H6). Hydrolysis of VI with 1 equivalent 2N NaOH gave 93% V. When a similar condensation was carried out by using 1 equivalent of NaOH in aqueous alc. 33% 5-(p-nitrophenoxy)pentyl glutaramate (VII), m. 93-5°(C6H6), was obtained identical with a specimen prepared in 34% yield from 5-(p-nitrophenoxy)pentyl bromide and Ag glutaramate in dry dioxane. Its structure was confirmed by catalytic reduction of VII to 81% 5-(p-aminophenoxy)pentyl glutaramate, m. 116-18°, and subsequent hydrolysis to 5-(p-aminophenoxy)pentanol, m. 94-5°. The following p-RC6H4O(CH2)nNHR1 (VIII) were prepared from IIa, 1-amino-4-(p-nitrophenoxy)butane, II, or 1-amino-8-(p-nitrophenoxy)octane with the appropriate acid chloride or anhydride either in C5H5N or under Schotten-Baumann conditions (n, R, R', % yield, m.p., and solvent of recrystn. given): 4, NO2, Bz, 82, 102-3°, aqueous AcOH; 5, NO2, p-BrC6H4CO, 81, 153-4°, alc.; 5, NO2, p-MeC6H4CO, 73, 132-3°, AcOH; 5, NO2, p-O2NC6H4CO, 49, 148-50°, Me2CO; 5, NO2, p-AcOC6H4CO, 54, 131-3°, Me2CO; 5, NO2, p-HOC6H4CO, 91, 147-50°, PhMe; 5, NO2, o-MeO2CC6H4CO, 61, 140-1°, C6H6; 5, NO2, p-MeO2CC6H4CO, 56, 164-6°, alc.; 5, NO2, p-MeSO2C6H4CO, 22, 169-71°, AcOH; 5, NO2, hexahydrobenzoyl, 87, 123°, AcOH; 5, NO2, EtCO, 69, 79-80°, aqueous alc.; 5, NO2, C5H11CO, 60, 59-60°, Et2O; 5, NO2, Ph2CHCO, 53, 104-6°, aqueous Me2CO; 5, NO2, Ph(CH2)4CO, 82, 87-9°, aqueous alc.; 5, NO2, 2,4-Cl2C6H3OCH2CO, 37, 112-14°, alc.; 5, NO2, C6H4(CO)2NCH2CO, 68, 183.5-5.0°, EtO(CH2)2OH; 5, AcNH, p-O2NC6H4CO, -, 214-17.5°, alc. or EtO(CH2)2OH; 8, NO2, PhSO2, 71, 73-5°, alc.; 5, NO2, p-MeC6H4SO2, 93, 154-6°, aqueous alc.; 5, NO2, p-AcNHC6H4SO2, 77, 129-31°, aqueous alc. N,N'-Bis[5-(p-nitrophenoxy)pentyl]terephthalamide (58%), m. 154-7° (alc.), and 39% N,N'-bis[5-(p-nitrophenoxy)pentyl]glutaramide, m. 127-9°(Me2CO), were similarly prepared II and NCCH2CO2Et in refluxing alc. gave 68% 1-cyanoacetamido-5-(p-nitrophenoxy)pentane, m. 85-6° (aqueous alc.). Similarly obtained in the absence of solvent was 73% N,N'-bis[5-(p-nitrophenoxy)pentyl]oxamide, m. 163.5-4.5° (CHCl3-alc.). Ethoxalyl chloride (13.65 g.) slowly added to 21.4 g. II in 100 ml. C5H5N, the solution kept overnight at room temperature, diluted with H2O and Et2O, and filtered gave 27% 1-ethoxalylamino-5-(p-nitrophenoxy)pentane, m. 85-7° (ligroine). II (36.4 g.), 13.95 ml. concentrated HCl, and 64.5 g. HCONH2 heated 0.5 hr. at 145°, cooled, evaporated, 100 ml. H2O added, and the crude product extracted with Et2O in a Soxhlet apparatus gave 78% 1-formamido-5-(p-nitrophenoxy)pentane, m. 71-2°. 2-Phenyloxazolone (8.2 g.) added to 12 g. II in CHCl3, the solvent evaporated, and the residue heated 0.5 hr. at 100° gave 80% 1-hippuramido-5-(p-nitrophenoxy)pentane, m. 145-7°(alc.). Ia (17.7 g.) refluxed 15 min. with 50 ml. N NaOH gave 1-(o-carboxybenzamido)-5-(p-

nitrophenoxy)pentane, m. 118-22° (CHCl3-ligroine). Tetra-Et pyrophosphate (2.7 ml.) added to 2.24 g. II and 1.79 g. p-acetamidobenzoic acid in 7 ml. di-Et phosphite, the mixture heated 1 hr. at 100°, diluted with H2O, and cooled gave 55% 1-(p-acetamidobenzamido)-5-(p-nitrophenoxy)pentane (IX), m. 187-8°(EtOCH2CH2OH). II (11.2 g.) added to 17.9 g. p-acetamidobenzoic acid and 9.52 g. p-MeC6H4SO2Cl in 40 ml. C5H5N, left 0.5 hr. at room temperature, and the mixture treated with 10 g. NaOH and 5 g. Na metabisulfite in 200 ml. H2O gave 60% IX. II (2.54 g.) in 10 ml. C5H5N refluxed 1.5 hrs. with 5 ml. BzCl gave 83% 1-dibenzoylamino-5-(p-nitrophenoxy)pentane, m. 119-20° (alc.). Benzyloxycarbonyl-β-alanine (24 g.) and 24 g. II in 75 ml. diethyl phosphite heated 0.5 hr. at 100° with 30 ml. tetraethyl pyrophosphite gave 90% 1-(N-benzyloxycarbonyl-β-alanylamino)-5-(p-nitrophenoxy)pentane (X), m. 137-8° (aqueous alc.). X (35.05 g.) left 20 min. with 60 ml. 33% HBr with evolution of CO2, the solution treated with Et2O, the hygroscopic hydrobromide filtered off, the salt dissolved in H2O, basified, and extracted with CHCl3 gave 1-(β-alanylamino)-5-(p-nitrophenoxy)pentane (XI), m. 93-5°(C6H6). XI (10.36 g.) and 4.56 g. DL-pantolactone in 50 ml. alc. refluxed 20 hrs., evaporated, and washed with 2N NaOH, 2N HCl, and H2O gave 14.6 g. 1-(p-nitrophenoxy)-5-(DL-pantothenamido)pentane, oil. 5-(p-Nitrophenoxy)pentyl bromide (XII) (43.2 g.) and 19.8 g. cyclohexylamine in 50 ml. alc. refluxed 19 hrs., cooled, and filtered gave 76% 1-cyclohexyl-amino-5-(p-nitrophenoxy)pentane-HBr, m. 221-3°(alc.); benzoyl derivative m. 78-9° (aqueous alc.). XII (44.5 g.) and 35 g. N-benzyloxybenzamide refluxed 24 hrs. with 3.5 g. Na and 300 ml. alc. gave 46% 1-(N-benzyloxybenzamido)-5-(p-nitrophenoxy)pentane, m. 77-8°. XII (57.6 g.), 50 ml. PhNH2, and 200 ml. alc. refluxed 20 hrs., concentrated, diluted with H2O, and crystallized gave 98% 1-anilino-5-(p-nitrophenoxy)pentane, m. 87-9° (alc.); Ac derivative noncryst.; methanesulfonyl derivative (XIII) (64%) m. 73-4° (C6H6-ligroine). XIII (42.7 g.), 5 ml. H2O, and 17.4 ml. MeI added to 3.5 g. Na in 300 ml. alc., the mixture refluxed 3 hrs., concentrated, and diluted with H2O gave 78% 1-(N-methylmethanesulfonamido)-5-(p-nitrophenoxy)pentane, m. 61-3°(Et2O). XII (28.8 g.) and 22.4 g. II in 250 ml. alc. refluxed 20 hrs. and the 68% crude HBr shaken with BzCl in Me2CO-2N NaOH gave 66% N-benzoylbis[4-(p-nitrophenoxy)pentyl]amine, m. 114-15.5° (Me2CO-Et2O). Condensation of K p-nitrophenoxide with 4-benzoylbutyl bromide in EtOCH2CH2OH gave 89% 1-benzoyl-4-(p-nitrophenoxy)butane (XIV), m. 122-3° (AcOH). XIV (63 g.) and 25.2 g. (iso-PrO)3Al in 3 l. iso-PrOH slowly distilled 2 hrs., the solution evaporated, and the residue treated with dilute HCl gave 94% 1-hydroxy-5-(p-nitrophenoxy)-1-phenylpentane (XV), m. 61-2° (aqueous alc.). PBr3 (21.6 ml.) added slowly under cooling at 10° to 54 g. XV in 500 ml. C6H6, the mixture kept overnight at room temperature, treated with H2O, the C6H6 layer separated, the aqueous layer extracted with Et2O, the combined organic layers dried, evaporated, the mixture refluxed 48 hrs. with 54 g. K phthalimide and 250 ml. Me2CO, and the product isolated gave 66% 5-(p-nitrophenoxy)-1-phenyl-1-phthalimidopentane (XVI), m. 131-2°(alc.). Hydrolysis of XVI with N2H4 and subsequent benzoylation afforded 69% 1-benzamido-5-(p-nitrophenoxy)-1-phenylpentane, m. 116-18°(C6H6). 1-(2-Hydroxyethoxy)-5-(p-nitrophenoxy)pentane was converted by p-MeC6H4SO2Cl in C5H5N into 81% p-toluenesulfonyl derivative, m. 49-50°, which condensed with K phthalide gave 65% 1-(p-nitrophenoxy)-5-(2-phthalimidoethoxy)pentane, m. 78-9° (MeOH). 5-(p-Nitrophenoxy)pentyl iodide (102 g.), 36 g. Na derivative of 2-pyridone, 400 ml. alc., and 200 ml. H2O refluxed 24 hrs. gave 47%

1-(1,2-dihydro-2-oxo-1-pyridyl)-5-(p-nitrophenoxy)pentane, m. 103° (Me2CO), and a small amount of 1-(p-nitrophenoxy)-5-(2-pyridyloxy)pentane. XII (2.88 g.), 1.73 g. Na derivative of 2,3-dihydro-3-oxobenzisothiazole (XVII), and 10 ml. EtOCH2CH2OH refluxed 20 hrs. gave 39% 1-(2,3-dihydro-3-oxobenzisothiazol-2-yl)-5-(p-nitrophenoxy)pentane, m. 109-11° (alc.). Oxidation with 30% H2O2 in AcOH at 100° gave the known saccharin derivative, m. 126-7°. XII (3.15 g.) condensed with 1.65 g. XVII by use of 0.76 g. K2CO3 in 50 ml. Me2CO gave 1.9 g. 1-(p-nitrophenoxy)-5(3-benzisothiazolyloxy)pentane, m. 97-9° (AcOH). CS2 (8.4 ml.) and 60 ml. HCONMe2 added successively to 32 g. II in 100 ml. PhMe, the mixture left 0.5 hr., cooled, shaken 0.5 hr. with 32 g. HgO, filtered, the filtrate treated with 7.3 g. 90% mercaptoacetic acid, the solution heated 0.5 hr. at 100°, concentrated, and diluted with Et2O gave 68% 3-[5-(p-nitrophenoxy)pentyl]rhodanine (XVIII), m. 112-13° (alc.). XVIII (30 g.) heated 3 hrs. at 100° with 20 ml. BzH, 200 ml. AcOH, and 40 ml. H2SO4 gave 96% 5-benzylidene derivative, m. 143-4° (AcOH). Thiazolidine-2,4-dione (14.1 g.) and 49.7 g. 5-(p-nitrophenoxy)pentyl iodide added successively to 3.43 g. Na and 200 ml. alc., the mixture refluxed 20 hrs., cooled, and filtered gave 46% 3-[5-(p-nitrophenoxy)pentyl]thiazolidine-2,4-dione, m. 118-19° (alc.). Butane-1,4-sultam (2 g.) in 0.35 g. Na and 10 ml. alc. and refluxed 3 hrs. with 4.3 g. XII in 10 ml. alc. gave 79% N-[5-(p-nitrophenoxy)pentyl]butane-1,4-sultam, m. 89-90° (MeOH). N-[5-(p-Nitrophenoxy)pentyl]naphthalene-1,8-sultam (59%) was similarly prepared from naphthalene-1,8-sultam, m. 1190 (alc.). 1-(p-Nitrophenoxy)-7-phthalimidoheptane (43.8 g.) reduced at 70°/56 lb./sq. in. in 350 ml. alc. over 2% PtO2 gave 55% 1-(p-aminophenoxy)-7-phthalimidoheptane, m. 107-9°. Concentration of the mother liquor gave 27% 1-(p-aminophenoxy)-7-hexahydrophthalimidoheptane, m. 73-5° (CHCl3-ligroine). 1-Maleimido-5-(p-nitrophenoxy)pentane (5.9 g.) kept 5 min. at 100° in 18 g. SnCl2.2H2O and 27 ml. concentrated HCl, poured into 50% NaOH and 100 ml. CHCl3 at 0°, the solution immediately separated, and crystallized gave 71% 1-(p-aminophenoxy)-5-maleimidopentane, m. 122-4° (EtOAcligroine); methanesulfonate m. 194-5°. 3-[5-(p-Aminophenoxy)pentyl]rhodanine (40%), m. 104-6° (alc.), and 73% 3-[5-(p-aminophenoxy)pentyl]-5-benzylidenerhodanine, m. 133-5° (AcOH), were similarly prepared 3-[5-(p-Aminophenoxy)pentyl]thiazolidine-2,4-dione was prepared in 54% yield by reducing the corresponding NO2 compound with SnCl2, or preferably with reduced Fe powder and aqueous AcOH, m. 107-9° (alc.). 1-Amino-5-(p-ami nophenoxy)pentane (14.55 g.), 8.36 g. CNCH2CO2Et, and 20 ml. MeOH kept 5 days gave 81% 1-(p-aminophenoxy)-5-(cyanoacetamido)pentane, m. 92-30 (alc.). The Ac derivative was obtained directly from 1-(p-acetamidophenoxy)-5-aminopentane and NCCH2CO2Et. Similarly prepared were 13% 1-(p-aminophenoxy)-5(dichloroacetamido)pentane, m. 81-2° (C6H6-ligroine), and 66% 1-(p-aminophenoxy)-5-(trichloroacetamido)pentane, m. 97-9° (Et2O). Concentrated HCl (100 ml.) added during 1 hr. to a refluxing mixture of 32.4 g. 1-(p-aminophenoxy)-5-phthalimidopentane (XVIIIa), 25 g. Sn, and 200 ml. alc., left 17 hrs., filtered, and the filtrate added to 200 ml. 50% NaOH gave 63% 1-(p-aminophenoxy)-5-phthalimidinopentane, m. 143-4°. Except where stated, the amines, p-H2NC6H4O(CH2)nR, were prepared by catalytic reduction of the corresponding NO2

compds., usually over Raney Ni in alc., EtOCH2CH2OH, or HCONMe2 (n, R, derivative, % yield, m.p., and solvent given): 2, phthalimido, base, 59, 159-60°, alc.; 2, phthalimido, McSO3H, -, 198-9°, -; 3, phthalimido, base, 94, 67-8° (or 92-3°), CHCl3-Et2O; 3, phthalimido, MeSO3H, -, 163-5°, EtOH-Et2O; 4, phthalimido, base, 59, 124-5°, alc.; 10, phthalimido, base, 70, 98°, alc.; 5,

tetrachlorophthalimido, base, 55, 180-2°, EtOCH2CH2OH; 5, 3-nitrophthalimido, base, 30, 117-18°, alc.; 5, 3-nitro phthalimido, MeSO3H, -, 183-5°, alc.-Et2O; 5, 3-aminophthalimido, base, 87, 105-7°, alc.; 5, homophthalimido, MeSO3H, 85, 187-9°, MeOH; 5, 3,4-dihydro-2,4-dioxo-5,6-benz-1,3-oxazin-3-yl, base, 95, 136-8°, alc.; 5, camphorimido, 0.5H2SO4, 54, 183-5°, alc.-Et2O; 5, 1,2,3,4-tetrahydro-11,4-dioxophthalazin-2-yl, base, 43, 169-71°, alc.; 5, glutarimido, base, 93, 109°, alc.; 5, β-ethyl-Bmethylglutarimido, base, 57, 99-100°, C6H6; 5, hexahydro-2,4,6-trioxopyrimidin-1-yl, base, 78, 211-14° (effervescent), Me2NCHO-alc.; 4, α-phthalimidobenzyl, base, 73, 112-13°, alc.; 4, α-benzamidobenzyl, MeSO3H, 63, 177-9°, alc.Et2O; 5, NHCHO, base, 89, 74-6°, C6H6; 5, NHCO2Et, base, 70, 77.5-9.0°, C6H6; 5, NHCOEt, CHPh:, -, 122.5-3.5°, -; 5, NHCOC5H11, base, 74, 86-7°, alc.Et2O; 5, NHCO(CH2)4Ph, base, 87, 92% CHCl3-ligroine; 5, NHCOCO2Et, base, 85, 78-80°, CHCl3-ligroine; 5, NHCOCO2Et, MeSO3H, -, 142-3°, alc.-Et2O; 5, NHCOCHPh2, base, 80, 101-2.5°, alc.-ligroine; 5, NHCOCH2C6H3Cl2-1,2,4, base, 84, 104.5-6.5°, alc.; 5, NHCOCH2N(CO2)C6H4-o, base, 98, 156.5-8.5°, alc.; 5, NHCOCH2NHCOPh, base, 81, 119-21°, alc.; 5, pantothenamido, base, 86, -, -; 5, hexahydrobenzamido, base, 85, 103-4°, C6H6; 5, N(COPh)2, base, 87, 92 3°, alc.; 4, NHCOPh, base, 80, 108°, alc.; 5, NHCOC6H4Me-p, base, 84, 123-4°, CHCl3-ligroine; 5, NHCOC6H4Br-p, base, 47, 118-20°, alc.; 5, NHCOC6H4Br-p, CHPh:, -, 154-5°, alc.; 5, NHCOC6H4OH-p, base, 67, 192.5-4.0°, alc.; 5, NHCOC6H4OH-o, base, 80, 122-3°, aqueous MeOH; 5, NHCOC6H4CO2Me-p, base, 77, 141-3°, PhMe; 5, NHCOC6H4CO2H-p, base, 93, 242-4°, aqueous HCONMe2; 5, NHCOC6H4SO2Me-p, base, 77, 144-5°, alc.; 5, NHCOC6H4NO2-p, base, 75, 139-41°, EtOAc; 5, NHCOC6H4NHAc-p, base, 89, 173.5-4.5°, alc.; 5, NHCOC6H4NH2-p, base, 80, 121-3°, alc.; 5, NHCOC6H4NH2-p, 2MeSO3H, -, 272-4°, alc.-Et2O; 5, NPhAc, base, 62, 66-8°, Et2O-ligroine; 5, N-cyclohexyl-benzamido, base, 80, 72-5°, Et2O-ligroine; 5, N(OCH2Ph)Bz, base, 96, 77-8°, aqueous alc.; 5, N(OH)Bz, base 78, 105-7°, alc.; 5, NBz(CH2)5OC6H4NH2-p, 2MeSO3H, 82, 137-9°, alc.-Et2O; 5, 1,2-dihydro-2-oxopyridyl, base, 96, 114-15°, alc.; 5, 2-oxopiperidino, base, 56, 97-8°, H2O; 5, 2,3-dihydro-3-oxobenzisothiazol-2-yl, base, 78, 117-19°, C6H6; 5, 2-phthalimidoethoxy, base, 94, 104-6°, alc.; 2, 4-phthalimidobut-1-enyl, base, -, 101-3°, aqueous alc.; 5, NHCONH (bis compound), base, 72, 160-2°, alc.; 5, NHCOCONH (bis compound), base, 79, 150-2°, EtOCH2CH2OH; 5, p-NHCOC6H4CONH (bis compound), base, 53, 176-8°, xylene; 5, NHCO(CH2)3 CONH (bis compound), base, 94, 133-5° and 140-1°, alc.; 5, NHCO(CH2)3CONH (bis compound), MeSO3H, -, 227-30°, alc.; 8, NHSO2Ph, base, 79, 121-2°, alc.; 5, NHSO2C6H4Me-p, base, 67, 168-9°, alc.; 5, NHSO2C6H4NHAc-p, base, 79, 117-19°, aqueous MeOH; 5, NHSO2C6H4NHAc-p, H2SO4, -, 198-201°, -; 5, NHSO2C6H4NH2-p, base, 64, 125-8°, aq.alc.; 5, NHSO2C6H4NH2-p, 2MeSO3H, -, 235-7°, -; 5, NPhSO2Me, base, 81, 67-8°, MeOH; 5, NMeSO2Me, base, 81, 76-7°, alc.-Et2O; 5, tetrahydro-1,1-dioxo-1,2-thiazin-2-yl, base, 60, 73°, Et2O; 5, 1,1-dioxonaphtho[1.8a.8-cd]isothiazol-2-yl, base, 92, 106-7°, alc. 1-(p-Aminophenoxy)-3-phthalimidopropane (m. 92-3°) converted to the MeI salt in 100% yield, m. 203-6° (H2O), and pyrolyzed under reduced pressure gave 100% 1-(p-dimethylaminophenoxy)-3-phthalimidopropane, m. 121-2°(alc.). 1-Benzenesulfonamido-5-(p-dimethylaminophenoxy)pentane, m. 71-2.5°

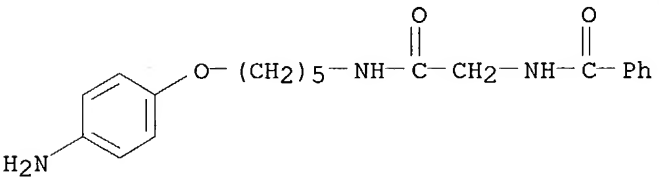
(Et2O), similarly obtained (96%) from its MeI salt (96%), m. 183-5° (H2O). p-(N-Methylacetamido)phenol, 5-phthalimidopentyl bromide, and NaOEt in alc. gave 53% 1-[p-(N-methylacetamido)phenoxy]-5-phthalimidopentane (XIX), m. 83-5° (CHCl3-Et2O). 1-[p-(N-Methylbenzamido)phenoxy]-5-phthalimidopentane, m. 121-4°(MeOH), was similarly obtained. Refluxing XIX with concentrated HCl gave 1-amino-5-(p-methylaminophenoxy)pentane, m. 76-9°(ligroine), decomposed on storage. The corresponding 5-phthalimido compound treated with aqueous alc.-N2H4 and the amine hydrolyzed gave 61% 1-benzamido-5-[p-(N-methylacetamido)phenoxy]pentane, m. 110-12° (Me2CO-ligroine). 1-Benzamido-5-[(p-(N methylformamido)phenoxy]pentane, m. 115-16° (Me2CO-Et2O), was similarly prepared in 12% yield. Partial hydrolysis of either the N-formyl or the N-Ac derivative with aqueous HCl gave 60% 1-benzamido-5-(p-methylaminophenoxy)pentane, m. 91-2° (Me2CO-ligroine); N-Bz derivative m. 111-13°(C6H6-Et2O). 1-Benzenesulfonamido-5-[p-(N-methylacetamido)phenoxy]pentane, m. 109-11° (PhMe-ligroine), was similarly prepared and was hydrolyzed to 62% 1-benzenesulfonamido-5-(p-methylaminophenoxy)pentane (XX), m. 83-5° (alc.). XX with HOCH2CH2Cl and CaCO3 in refluxing H2O gave 76% 1-benzenesulfonamido-5-[p-(2-hydroxy-N-methylethylamino)phenoxy]pentane, m. 76-8° (C6H6-ligroine). 1-(p-Aminophenoxy)-5-benzamidopentane (XXa) (14.9 g.), 4.7 g. (CH2Br)2, and 25 ml. alc. refluxed 20 hrs. gave 3.3 g. piperazine derivative and 24% 1,2-bis[p-(5-benzamidopentyloxy)anilino]ethane (XXI), m. 155-7°(alc.). XXI (8.1 g.), 4.7 g. (CH2Br)2, and 4.2 g. NaHCO3 refluxed 20 hrs. in 30 ml. EtOCH2CH2OH gave 1,4-bis[p-(5-benzamidopentyloxy)phenyl]piperazine, m. 231-3°(EtOCH2CH2OH). POCl3 (2.74 g.) added to 4.12 g. 1-[p-bis(2-hydroxyethyl)aminophenoxy]-5-phthalimidopentane in 15 ml. C6H6, the mixture refluxed 2 hrs., poured on ice, and extracted with C6H6 gave 81% 1-[p-bis(2-chloroethyl)aminophenoxy]-5-phthalimidopentane (XXII), m. 107-8° (alc.). XXII (17.96 g.), 5.66 g. 3-chloro-p-toluidine, 4.24 g. Na2CO3, and 75 ml. EtOCH2CH2OH refluxed 20 hrs. gave 63% 1-(3-chloro-p-tolyl)-4-[p-(5-phthalimidopentyloxy)phenyl]piperazine, m. 149-50° (CHCl3-alc.). 2-Amino-4-chloro-6-methylpyrimidine (14.35 g.), 32.4 g. XVIIIa, 100 ml. N HCl, and 500 ml. H2O refluxed 1 hr., and made alkaline gave 67% 1-[p-(2-amino-6-methylpyrimid-4-ylamino)phenoxy]-5-phthalimidopentane, m. 211-13° (EtOCH2CH2OH); 1-methomethylsulfate (75%) m. 186-8° (alc.). NaNO2 (91.43 g.) in 24 ml. H2O added slowly at 0-5° to 4.16 g. p-aminobenzamidine-2HCl and 2.9 ml. concentrated HCl in 17 ml. H2O, 6.28 g. XVIIIa in 20 ml. AcOH added quickly followed by NaOAc, and the product separated gave 68% 4-amidino-4'-[(5-phthalimido)pentyloxydiazoamino]benzene acetate, m. 210-12°(alc.). XXa (19.7 g.), 6.18 g. chloracetamide, 3.5 g. Na2CO3, and 200 ml. alc. refluxed 20 hrs. gave 61% 5-benzamido-1 (p-carbamoylmethylaminophenoxy)pentane, m. 161-3° (alc.). XVIIIa (3.24 g.), 1.8 g. D-glucose, and 0.5 ml. 5% alc. CaCl2 in 20 ml. alc. refluxed 1.5 hrs. gave 86% 1-(p-D-glucosylaminophenoxy)-5-phthalimidopentane, m. 110-15°. 1-Benzamido-5-(p-D-glucosylamino)pentane (83%) was similarly prepared, m. 119-20° (aqueous MeOH). IIIa (14.6 g.), 10.65 g. 1-(3-chloro-p-tolyl)piperazine, and 75 ml. alc. refluxed 40 hrs. gave 76% 4-(3-chloro-p-tolyl) 1-[5-(p-nitrophenoxy)pentyl]piperazine (XXIII).HBr, m. 170-2°(alc.). Free XXIII m. 101-3°(alc.). Reduction of XXIII with Na2S gave 86% 1-[5-(p-aminophenoxy)pentyl]-4-(3-chloro-p-tolyl)piperazine, m. 95-6° (alc.). IIIa (5.76 g.) and 1.94 g. piperazine-6H2O heated 40 hrs. at 100° and the residue refluxed with alc. gave 92% 1,4-bis[5-(p-nitrophenoxy)pentyl]piperazine-2HBr, m. 253-5°; free base m. 122-3° (alc.). Catalytic reduction gave

92% 1,4-bis[5-(p-aminophenoxy)pentyl]piperazine, m. 124-6° (alc.-ligroine). The following RC6H4O(CH2)5R' were prepared (R, R', m.p., and solvent for recrystn. given): p-NHCHO, NHBz, 163-4°, alc.; p-NHAc, NHBz, 165-7°, alc.; p-NHAc, NHAc, 155-7°, H2O; p-HO2C(CH2)2CONH, o-C6H4(CO)2N, 185-7°, AcOH; p-NH4O2C(CH2)2CONH, o-C6H4(CO)2N, 174-6°, -; p-(5-nitrofurfurylidene)amino, o-C6H4(CO)2N, 138-9°, CHCl3-alc.; p-PhCH:N, NHBz, 133-4° alc.; p-MeN(NO), o-C6H4(CO)2N, 104-5°, alc.; o-NO2, o-C6H4(CO)2N, 99.5°, alc.; o-NH2, o-C6H4(CO)2N, 94-5°, alc.; m-NHAc, o-C6H4(CO)2N, 127.5-9.0°, alc.; m-NH2, o-C6H4(CO)2N, 102-3°, alc.

IT **103388-58-5**, Benzamide, N-{{[5-(p-aminophenoxy)pentyl]carbamoyl}methyl}- **117123-84-9**, Benzamide, N-{{[5-(p-nitrophenoxy)pentyl]carbamoyl}methyl}-
(preparation of)

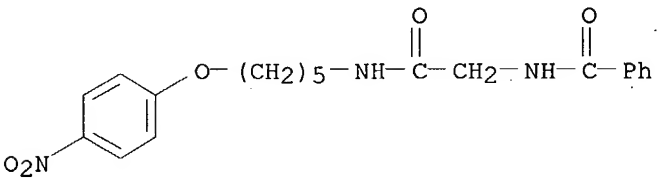
RN 103388-58-5 CAPLUS

CN Benzamide, N-[[[5-(p-aminophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)

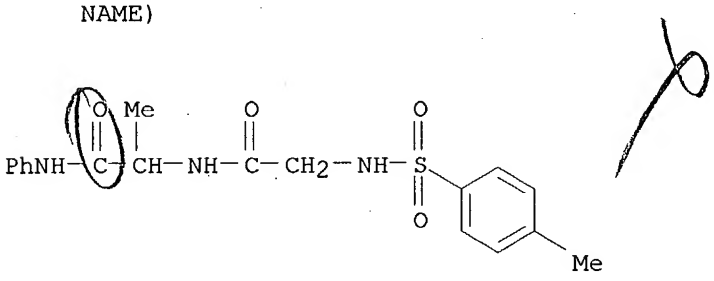


RN 117123-84-9 CAPLUS

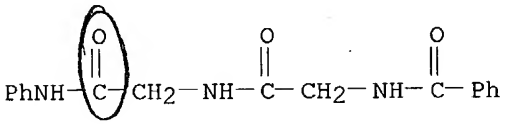
CN Benzamide, N-[[5-(p-nitrophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



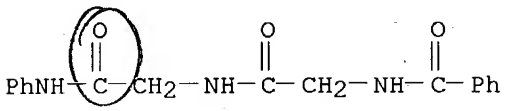
L71 ANSWER 44 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1960:11409 CAPLUS
DN 54:11409
OREF 54:2312d-h
TI Aminolysis of 1-acyl-3,5-dimethylpyrazoles
AU Ried, Walter; Schleimer, Bernhard
CS Univ. Frankfurt, Germany
SO Ann. (1959), 626, 98-105
DT Journal
LA Unavailable
OS CASREACT 54:11409
AB The aminolysis of a number of 1-acyl-3,5-dimethylpyrazoles was studied as a function of the acyl group, the basicity of the aminolyzing base, and the nature of the solvent. By condensation of the corresponding acid hydrazide with acetylacetone in the heat, reaction of the acid hydrazide with acetylacetone in aqueous HCl at room temperature, or reaction of 3,5-dimethylpyrazole with the acid chloride were prepared 1-acyl-3,5-dimethylpyrazoles with the following acyl groups: Ac (b12 70°), COCH2CN (m. 118-21°), COCH2SH (m. 118-19.5°), COCH2Cl (m. 68-70°), COCH2OPh (m. 85-7°), COCH2Ph (m. 56.5-58°), Bz (b12 158°), COC6H4NO2-p (m. 122.5-3.5°), COC6H4NH2-p (m. 95.5-6.5°), OCNH2 (m. 112-13°), SO2C6H4Me-p (m. 96.5-7.5°), N-tosylglycyl (m. 119-20.5°), N-tosyl-DL-alanyl (m. 144.5-5.5°), N-tosyl-DL-valyl (m. 149.5-50.5°), N-tosylglycyl-DL-alanyl (m. 143.5-4.5°), N-tosyl-L-leucyl (m. 164-6°), and N-tosyl-L-tyrosyl (m. 165-6°). Electropos. substituents in the acyl component lowered the reaction rate of aminolysis, electroneg. ones increased it. Thus, 1-(p-nitrobenzoyl)-3,5-dimethylpyrazole was very easily aminolyzed by aniline, while even at temps. up to 180° 1-(p-aminobenzoyl)-3,5-dimethylpyrazole was not. Of the pyrazoles containing the tosyl group only the 1-tosyl- and 1-(N-tosyl-DL-valyl)-3,5-dimethylpyrazole could not be aminolyzed by aniline. N-Tosylglycyl- (m. 159-60°), N-tosyl-DL-alanyl- (m. 163-4.5°), N-tosylglycyl-DL-alanyl- (m. 1567.5°), and N-tosyl-L-tyrosylanilide (m. 183-5°) were obtained in this manner from the corresponding 1-(N-tosyl-α-aminoacyl)-3,5-dimethylpyrazoles. Glacial AcOH exerted an effect on the aminolysis reaction similar to that of positivating group in the acyl component. Thus, in benzene, 1-cyanoacetyl-3,5-dimethylpyrazole was not aminolyzed by benzaldehyde phenylhydrazone, while in glacial AcOH N-cyanoacetyl-N-phenyl-N'-benzylidenehydrazine (m. 201-3°) was obtained in good yields. N-Cyanoacetyl-N-phenyl-N'-(p-nitrobenzylidene)hydrazine (m. 205-7°) was prepared similarly.
IT **101720-38-1**, Propionanilide, 2-(2-p-toluenesulfonamidoacetamido)- (preparation of)
RN 101720-38-1 CAPLUS
CN Propionanilide, 2-(2-p-toluenesulfonamidoacetamido)- (6CI) (CA INDEX NAME)



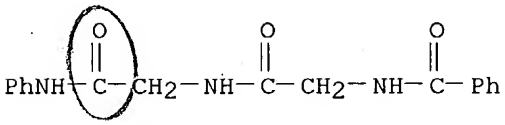
L71 ANSWER 45 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1959:76148 CAPLUS
DN 53:76148
OREF 53:13774g-i
TI Ultraviolet absorption spectra of benzoyl polyglycine anilides and benzoyl polyalanine anilides
AU Goldfarb, A. R.; Hoffmann, E.
CS Chicago Med. School
SO Archives of Biochemistry and Biophysics (1959), 81, 493-9
CODEN: ABBIA4; ISSN: 0003-9861
DT Journal
LA Unavailable
AB cf. C.A. 52, 20318f. Benzoyldiglycine (1.2 g.) dispersed in 10 ml. $CHCl_3$, the mixture treated with 0.71 ml. Et_3N, cooled (ice bath), 0.39 ml. $ClCO_2Me$ added, the mixture stirred 15-20 min., treated with 0.46 ml. $PhNH_2$, allowed to warm to room temperature during a few hrs., held overnight at room temperature, evaporated to dryness, and the residue washed with H_2O, dilute alkali, dilute acid, and H_2O yielded 1 g. benzoyl diglycine anilide, m. 248°. Other glycine and alanine anilides were prepared by the same method. The absorption spectra of the compds. were studied in MeOH and $HClO_4$. The data support the hypothesis that interactions between peptide bonds occur which are energetic in nature.
IT **93818-92-9**, Acetanilide, 2-(2-benzamidoacetamido)- (spectrum of)
RN 93818-92-9 CAPLUS
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



L71 ANSWER 46 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1957:47458 CAPLUS
DN 51:47458
OREF 51:8846c-d
TI Enzymic synthesis of peptide bonds. VII. Competition between some benzoylamino acids and benzoyldipeptides in papain-catalyzed reactions with glycinanilide
AU Tollin, Gordon; Fox, Sidney W.
CS Florida State Univ., Tallahassee
SO Archives of Biochemistry and Biophysics (1957), 66, 411-17
CODEN: ABBIA4; ISSN: 0003-9861
DT Journal
LA Unavailable
AB cf. C.A. 48, 2148b. A series of competition expts. in which more than one benzoylamino acid or benzoyldipeptide component was present with glycinanilide and papain were performed. In some reactions, the product represented the faster-reacting component; in others it did not. The 2nd component, in the latter instances, altered the normal course of the reaction. The theory of the participation of proteases in protein synthesis is discussed.
IT **93818-92-9**, Acetanilide, 2-(2-benzamidoacetamido)-
(formation from glycinanilide by papain)
RN 93818-92-9 CAPLUS
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



L71 ANSWER 47 OF 47 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1954:11568 CAPLUS
DN 48:11568
OREF 48:2148b-e
TI Enzymic synthesis of peptide bonds. VI. The influence of residue type on papain-catalyzed reactions of some benzoylamino acids with some amino acid anilides
AU Fox, Sidney W.; Winitz, Milton; Pettinga, Cornelius W.
CS Iowa State Coll., Ames
SO Journal of the American Chemical Society (1953), 75, 5539-42
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB cf. C.A. 47, 5465d. Each of 13 benzoylamino acids was submitted to reaction with glycinanilide in the presence of papain. Only benzoylglycine (I) participated in a synthesis leading to a larger peptide. The failure of benzoylaminoisobutyric acid to react is explainable on the basis of steric hindrance. Benzoylglutamic acid and benzoyltyrosine did not react at pH values in which the corresponding reactions with PhNH2 had been shown to proceed rapidly. Eight other reactions were transacylations yielding glycine-free products. I with each of 4 amino acid anilides yielded benzoylglycylamino acid anilide. When benzoylalanine was used instead of I, 2 syntheses and 2 transacylations resulted. The acylamino acid and the amino acid anilide thus each contribute to selectivity in synthesis. The specificities observed when the carboxoid or aminoid component is systematically varied contrasts, at the 2 amino acid level, with the broad preferences observed in reactions of benzoylamino acid with PhNH2. A single protease participating in peptide-bond synthesis may favor unique synthetic reactions, and reject or divert others. These phenomena are referred to as zymosequential specificity. These observations suggest the possibility that, in protein synthesis, each peptide intermediate becomes part of the protease to give, in effect, a new enzyme at each step.
IT **93818-92-9**, Acetanilide, 2-(2-benzamidoacetamido)-
(preparation of)
RN 93818-92-9 CAPLUS
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



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L65             SCREEN 2016 OR  2026 OR  2039 OR  2040 OR  2045 OR  2047
L66             STRUCTURE UPLOADED
L67             QUE L66 AND L64 NOT L65
L68           0 S L67 SSS SAM
L69           0 S L62 SSS SAM
L70          67 S L62 SSS FUL

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     FILE 'CAOLD' ENTERED AT 17:53:26 ON 16 JUN 2004

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L72          10 L70

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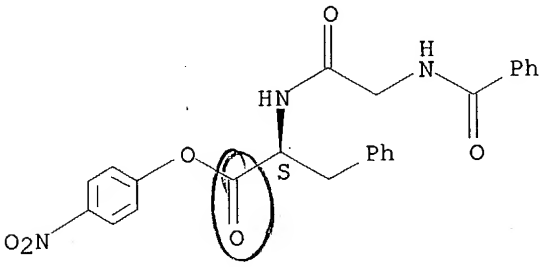
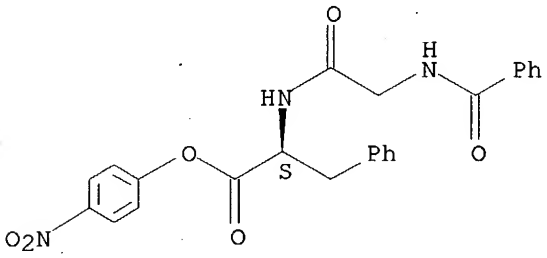
L72 ANSWER 1 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA63:16450d CAOLD
TI racemization
AU Young, Geoffrey T.; Antonovics, I.
IT **2900-37-0**
RN 2900-37-0 CAOLD
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.

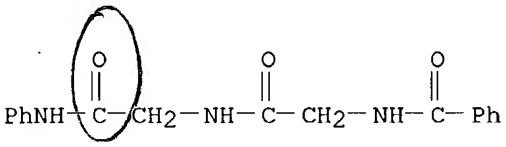


L72 ANSWER 2 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA63:14976h CAOLD
TI synthesis of peptides related to eledoisin
AU Boissonnas, Roger A.; Sandrin, E.
IT **2900-37-0**
RN 2900-37-0 CAOLD
CN Alanine, N-hippuroyl-3-phenyl-, p-nitrophenyl ester, L- (8CI) (CA INDEX NAME)

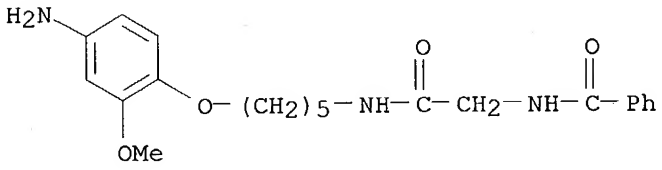
Absolute stereochemistry.



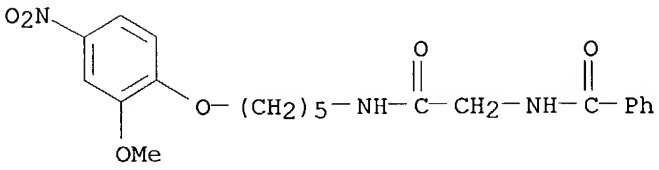
L72 ANSWER 3 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA56:6084c CAOLD
TI reactions of formylamino acids and acyldipeptides with dicyclohexylcarbodiimide
AU Siemion, Ignacy Z.; Nowak, K.
IT **93818-92-9**
RN 93818-92-9 CAOLD
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



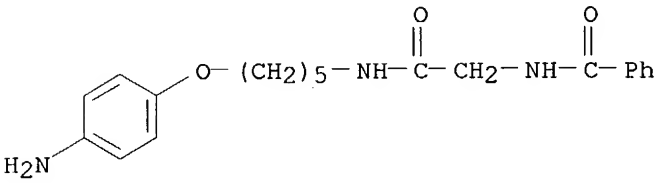
L72 ANSWER 4 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA55:21020b CAOLD
IT **103506-85-0**
RN 103506-85-0 CAOLD
CN Benzamide, N-[[[5-(4-amino-2-methoxyphenoxy)pentyl]carbamoyl]methyl]-
(6CI) (CA INDEX NAME)



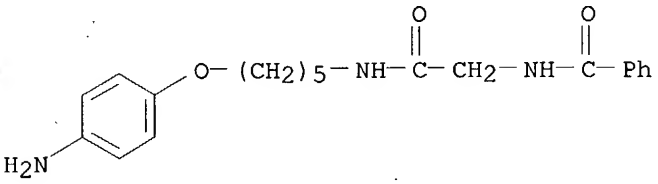
L72 ANSWER 5 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA55:21015i CAOLD
TI chemotherapy of schistosomiasis - (IV) ethers of 4-amino-2-methoxyphenol
AU Collins, Raymond F.; Davis, M.
IT **103990-63-2**
RN 103990-63-2 CAOLD
CN Benzamide, N-[[[5-(2-methoxy-4-nitrophenoxy)pentyl]carbamoyl]methyl]-
(6CI) (CA INDEX NAME)



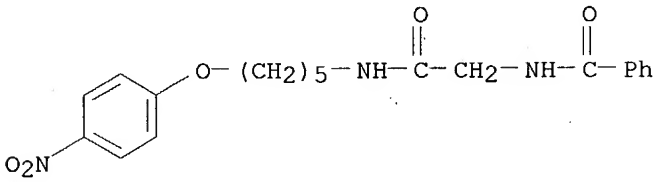
L72 ANSWER 6 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA54:16655b CAOLD
TI schistosomicidal and toxic effects of some N-p-aminophenoxyalkylamides
AU Collins, Raymond F.; Davis, M.; Edge, N. D.; Hill, J.; Reading, H. W.; Turnbull, E. R.
IT **103388-58-5**
RN 103388-58-5 CAOLD
CN Benzamide, N-[[[5-(p-aminophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



L72 ANSWER 7 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA54:7613f CAOLD
TI chemotheraphy of schistosomiasis - (III) N-(p-aminophenoxyalkyl)amides, -imides, and -sulfonamides
AU Ashley, Julius N.; Collins, R. F.; Davis, M.; Sirett, N. E.
IT **103388-58-5 117123-84-9**
RN 103388-58-5 CAOLD
CN Benzamide, N-[[[5-(p-aminophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



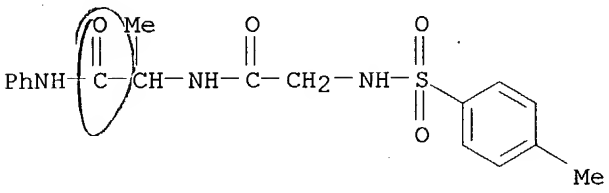
RN 117123-84-9 CAOLD
CN Benzamide, N-[[5-(p-nitrophenoxy)pentyl]carbamoyl]methyl]- (6CI) (CA INDEX NAME)



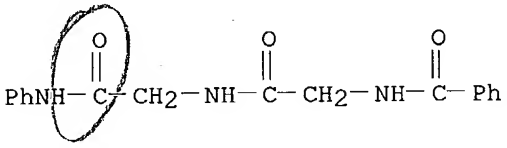
L72 ANSWER 8 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA54:2312d CAOLD
TI aminolysis of 1-acyl-3,5-dimethylpyrazoles
AU Ried, Walter; Schleimer, B.

PATENT NO.	KIND	DATE
DE 1054968		

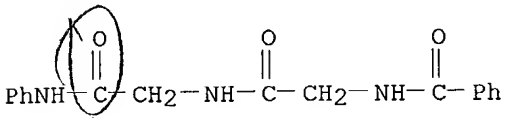
IT **101720-38-1**
RN 101720-38-1 CAOLD
CN Propionanilide, 2-(2-p-toluenesulfonamidoacetamido)- (6CI) (CA INDEX NAME)



L72 ANSWER 9 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA53:13774g CAOLD
TI ultraviolet absorption spectra of benzoyl polyglycine anilides and benzoyl polyalanine anilides
AU Goldfarb, A. R.; Hoffmann, E.
IT **93818-92-9**
RN 93818-92-9 CAOLD
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



L72 ANSWER 10 OF 10 CAOLD COPYRIGHT 2004 ACS on STN
AN CA51:8846c CAOLD
TI enzymic synthesis of peptide bonds - (VII) competition between benzoylamino acids and benzoyldipeptides in papain-catalyzed reactions with glycinanilide, (VIII) activation phenomena in the papsin-catalyzed synthesis of peptide bonds
AU Tollin, Gordon; Fox, S. W.
IT **93818-92-9**
RN 93818-92-9 CAOLD
CN Acetanilide, 2-(2-benzamidoacetamido)- (6CI, 7CI) (CA INDEX NAME)



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